

10/529,895

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PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 20:41:06 ON 19 JUN 2008
FILE 'CAPLUS' ENTERED AT 20:41:06 ON 19 JUN 2008
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	12.82	369.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.60	-1.60

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	12.82	369.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.60	-1.60

FILE 'REGISTRY' ENTERED AT 20:41:16 ON 19 JUN 2008
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provided by InfoChem.

STRUCTURE FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9
DICTIONARY FILE UPDATES: 18 JUN 2008 HIGHEST RN 1029146-45-9

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10529895claim23.str

L7 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10529895b.str

L8 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10529895a.str

L9 STRUCTURE UPLOADED

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=> s 17

SAMPLE SEARCH INITIATED 20:42:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12079 TO ITERATE

16.6% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 234994 TO 248166
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L7

=> s 17 full

FULL SEARCH INITIATED 20:42:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 242270 TO ITERATE

100.0% PROCESSED 242270 ITERATIONS 40 ANSWERS
SEARCH TIME: 00.00.02

L11 40 SEA SSS FUL L7

=> s 18

SAMPLE SEARCH INITIATED 20:42:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 45 TO ITERATE

100.0% PROCESSED 45 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 498 TO 1302
PROJECTED ANSWERS: 6 TO 266

L12 6 SEA SSS SAM L8

=> s 18 full

FULL SEARCH INITIATED 20:43:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1100 TO ITERATE

100.0% PROCESSED 1100 ITERATIONS 136 ANSWERS
SEARCH TIME: 00.00.01

L13 136 SEA SSS FUL L8

=> s 19

SAMPLE SEARCH INITIATED 20:43:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 45 TO ITERATE

100.0% PROCESSED 45 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 498 TO 1302
PROJECTED ANSWERS: 0 TO 0

L14 0 SEA SSS SAM L9

=> s 19 full

FULL SEARCH INITIATED 20:43:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1100 TO ITERATE

100.0% PROCESSED 1100 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L15 1 SEA SSS FUL L9

=> d his

(FILE 'HOME' ENTERED AT 19:31:27 ON 19 JUN 2008)

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FILE 'REGISTRY' ENTERED AT 19:31:48 ON 19 JUN 2008
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 STRUCTURE UPLOADED
L4 3 S L1 FULL
L5 0 S L3 FULL

FILE 'CAPLUS' ENTERED AT 19:32:55 ON 19 JUN 2008
L6 2 S L4

FILE 'REGISTRY' ENTERED AT 20:41:16 ON 19 JUN 2008
L7 STRUCTURE UPLOADED
L8 STRUCTURE UPLOADED
L9 STRUCTURE UPLOADED
L10 0 S L7
L11 40 S L7 FULL
L12 6 S L8
L13 136 S L8 FULL
L14 0 S L9
L15 1 S L9 FULL

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	536.46	906.21
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.60

FILE 'CAPLUS' ENTERED AT 20:44:47 ON 19 JUN 2008
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FILE COVERS 1907 - 19 Jun 2008 VOL 148 ISS 25
FILE LAST UPDATED: 18 Jun 2008 (20080618/ED)

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=> s l11
L16 13 L11

=> s l13
L17 3 L13

=> s l15
L18 1 L15

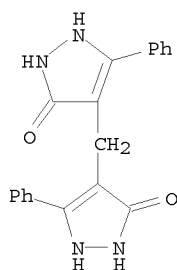
=> s l16 or l17 or l18
L19 13 L16 OR L17 OR L18

=> d bib abs hitstr 1-13 l19

L19 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:488218 CAPLUS
DN 148:202632
TI 4-[(3-Hydroxy-5-phenyl-1H-pyrazol-4-yl)methyl]-5-phenyl-1H-pyrazol-3(2H)-

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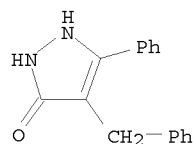
one
 AU Baryala, Yamna; Zerzouf, Abdelfettah; Essassi, El Mokhtar; Reuter, Hans; Eickmeier, Henning
 CS Laboratoire de Chimie Organique et Etudes Physicochimiques, ENS Rabat, Morocco
 SO Acta Crystallographica, Section E: Structure Reports Online (2007), E63(5), o2554-o2556
 CODEN: ACSEBH; ISSN: 1600-5368
 URL: <http://journals.iucr.org/e/issues/2007/05/00/fj2013/fj2013.pdf>
 PB Blackwell Publishing Ltd.
 DT Journal; (online computer file)
 LA English
 AB The solid-state structure of 4-[(3-hydroxy-5-phenyl-1H-pyrazol-4-yl)methyl]-5-phenyl-1H-pyrazol-3(2H)-one, C₁₉H₁₆N₄O₂, is dominated by the keto-enol tautomerization of its 2 1H-pyrazol-3-one moieties. Since all H atoms could be located in a difference Fourier synthesis, it was possible to distinguish the enol form from the keto form unambiguously. Of this tautomerization, an intramol. H bond embedded in an 8-membered ring is formed. The 2-dimensional H-bonding system results from 3 addnl. intermol. H bonds of different strengths, all involved in 8- and 10-membered ring systems. Crystallog. data are given.
 IT 1003355-45-0P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal and mol. structure of)
 RN 1003355-45-0 CAPLUS
 CN 3H-Pyrazol-3-one, 4,4'-methylenebis[1,2-dihydro-5-phenyl- (CA INDEX NAME)]



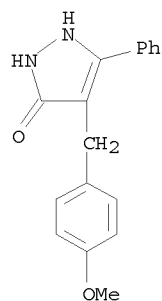
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2005:573840 CAPLUS
 DN 143:229781
 TI Selective reduction of the exocyclic double bond of isoxazolones and pyrazolones by hantzsch 1,4-dihydropyridine
 AU Liu, Zhengang; Han, Bing; Liu, Qiang; Zhang, Wei; Yang, Li; Liu, Zhong-Li; Yu, Wei
 CS National Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China
 SO Synlett (2005), (10), 1579-1580
 CODEN: SYNLES; ISSN: 0936-5214
 PB Georg Thieme Verlag
 DT Journal
 LA English
 OS CASREACT 143:229781
 AB Hantzsch 1,4-dihydropyridine (HEH) was used to realize the selective reduction of the exocyclic double bond of 4-arylmethylene- and 4-alkylidene-4H-isoxazol-5-ones and 4-arylmethylene-4H-pyrazol-5-ones.
 IT 500584-63-4P 863037-49-4P 863037-51-8P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of [(aryl)alkyl]pyrazolone derivs. by selective reduction of exocyclic double bond of [(aryl)methylene]pyrazolone derivs. using Hantzsch 1,4-dihydropyridine)
 RN 500584-63-4 CAPLUS
 CN 3H-Pyrazol-3-one, 1,2-dihydro-5-phenyl-4-(phenylmethyl)- (CA INDEX NAME)

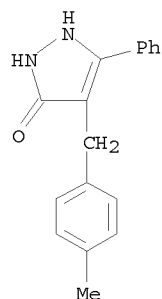
10/529,895



RN 863037-49-4 CAPLUS
CN 3H-Pyrazol-3-one, 1,2-dihydro-4-[(4-methoxyphenyl)methyl]-5-phenyl- (CA
INDEX NAME)



RN 863037-51-8 CAPLUS
CN 3H-Pyrazol-3-one, 1,2-dihydro-4-[(4-methylphenyl)methyl]-5-phenyl- (CA
INDEX NAME)



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:1156566 CAPLUS
DN 142:94061
TI Preparation of pyrazole glycoside compounds as SGLT inhibitors
IN Kikuchi, Norihiko; Fujikura, Hideki; Tazawa, Shigeki; Yamato, Tokuhisa;
Isaji, Masayuki
PA Kissei Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

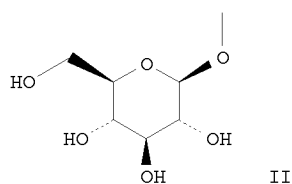
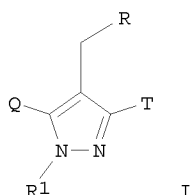
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004113359	A1	20041229	WO 2004-JP8695	20040615
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,			

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AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

CA 2529878	A1	20041229	CA 2004-2529878	20040615
EP 1637539	A1	20060322	EP 2004-746165	20040615
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
US 20070060531	A1	20070315	US 2006-561217	20061113
PRAI JP 2003-175663	A	20030620		
WO 2004-JP8695	W	20040615		
OS MARPAT 142:94061				
GI				



AB Title compds. I [R1 = H, (un)substituted alkyl, etc.; one of Q and T is II, etc.; the other is Z-Ar; Z = O, etc.; Ar = aryl, etc.; R = (un)substituted cycloalkyl, etc.] were prepared For example, glycosidation of 1-isopropyl-4-(4-methoxybenzyl)-5-phenoxy-1,2-dihydro-3H-pyrazol-3-one by 2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl bromide in the presence of benzyltributylammonium chloride followed by deacetylation using sodium methoxide afforded compound I [R1 = isopropyl; R = 4-methoxyphenyl; Q = phenoxy; T = II]. In SMINT inhibition assays, the IC50 value of compound I [R1 = isopropyl; R = 4-methoxyphenyl; Q = phenoxy; T = II] was 700 nM. Of note, compds. I have SGLT inhibition activity (no data provided). Compds. I are claimed useful for the treatment of diabetes, obesity, etc.

IT 815581-51-2P 815581-53-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazole glycoside compds. as SGLT inhibitors for treatment of diabetes and obesity)

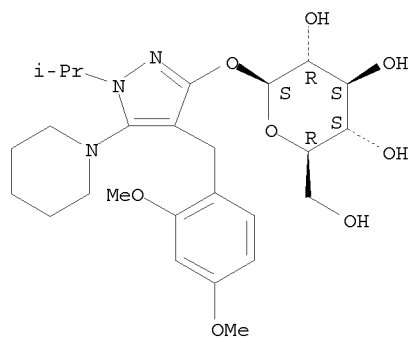
RN 815581-51-2 CAPLUS

CN β-D-Glucopyranoside, 4-[(2,4-dimethoxyphenyl)methyl]-1-(1-methylethyl)-5-(1-piperidinyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

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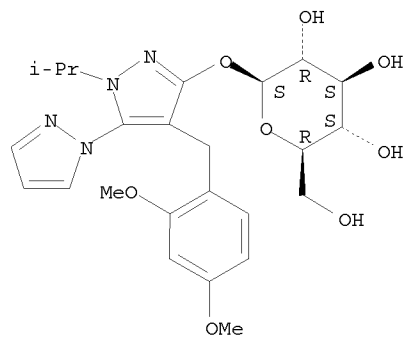
10/529,895



RN 815581-53-4 CAPLUS

CN β -D-Glucopyranoside, 4'-[(2,4-dimethoxyphenyl)methyl]-1'-(1-methylethyl)[1,5'-bi-1H-pyrazol]-3'-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



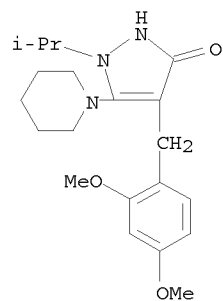
IT 815581-63-6P 815581-64-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrazole glycoside compds. as SGLT inhibitors for treatment of diabetes and obesity)

RN 815581-63-6 CAPLUS

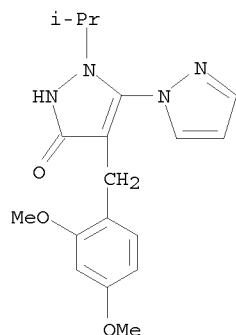
CN 3H-Pyrazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-1,2-dihydro-1-(1-methylethyl)-5-(1-piperidinyl)- (CA INDEX NAME)



RN 815581-64-7 CAPLUS

CN [1,3'-Bi-1H-pyrazol]-5'(2'H)-one, 4'-[(2,4-dimethoxyphenyl)methyl]-2'-(1-methylethyl)- (CA INDEX NAME)

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RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:486406 CAPLUS

DN 141:47334

TI Preventive or remedy for diseases caused by hyperglycemia

IN Ito, Fumiaki; Shibazaki, Toshihide; Tomae, Masaki; Fushimi, Nobuhiko;
Isaji, Masayuki

PA Kissei Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DT Patent

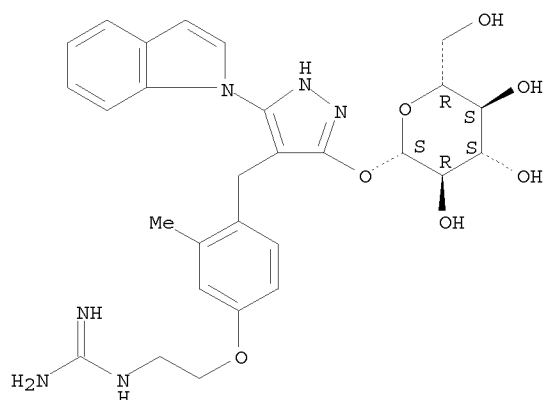
LA Japanese

FAN.CNT 1

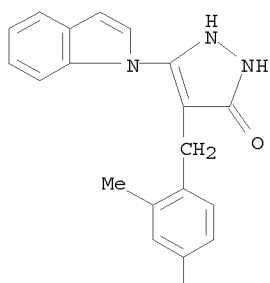
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004050122	A1	20040617	WO 2003-JP15503	20031204
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2507665	A1	20040617	CA 2003-2507665	20031204
AU 2003289156	A1	20040623	AU 2003-289156	20031204
EP 1568380	A1	20050831	EP 2003-777222	20031204
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
CN 1744916	A	20060308	CN 2003-80109504	20031204
US 20060035844	A1	20060216	US 2005-537495	20050603
IN 2005DN02385	A	20070105	IN 2005-DN2385	20050603
PRAI JP 2002-352201	A	20021204		
WO 2003-JP15503	W	20031204		
AB	It is intended to provide a medicinal composition containing as the active ingredient a selective SGLT1 inhibitor (for example, an SGLT1 inhibitor substantially showing no GLUT2 and/or GLUT5 inhibitory effect) which exerts a sugar absorption inhibitory effect over a wide range, also has a hypoglycemic effect caused by fructose intake in usual diet and thus can show an outstanding hypoglycemic effect and which is appropriate as a preventive or a remedy for diseases caused by hyperglycemia (for example, diabetes, impaired glucose tolerance, diabetic complications or obesity).			
IT	705445-35-8P, 3-(β-D-Glucopyranosyloxy)-4-[[4-(2-guanidinoethoxy)-2-methylphenyl]methyl]-5-indolyl-1H-pyrazole			
RL:	PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)			
	(SGLT1 inhibitors as preventives or remedies for diseases caused by hyperglycemia)			
RN	705445-35-8 CAPLUS			
CN	Guanidine, [2-[4-[[3-(β-D-glucopyranosyloxy)-5-(1H-indol-1-yl)-1H-pyrazol-4-yl]methyl]-3-methylphenoxy]ethyl]- (9CI) (CA INDEX NAME)			

10/529,895

Absolute stereochemistry.



IT 705445-10-9P 705445-15-4P 705445-20-1P
705445-25-6P, 3-(2,3,4,6-Tetra-O-acetyl-β-D-glucopyranosyloxy)-4-[[4-(2-acetoxyethoxy)-2-methylphenyl]methyl]-5-indolyl-1H-pyrazole 705445-30-3P 705445-45-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(SGLT1 inhibitors as preventives or remedies for diseases caused by hyperglycemia)
RN 705445-10-9 CAPLUS
CN 3H-Pyrazol-3-one, 1,2-dihydro-5-(1H-indol-1-yl)-4-[[2-methyl-4-[2-(phenylmethoxy)ethoxy]phenyl]methyl]- (CA INDEX NAME)



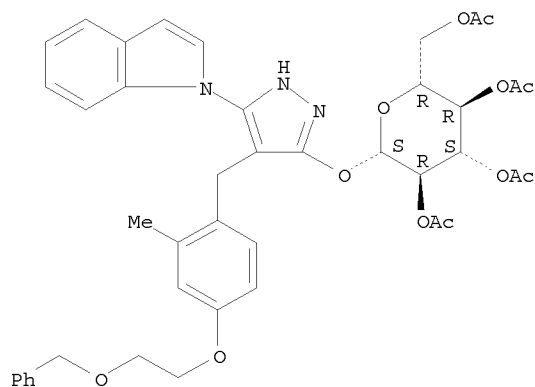
Ph-CH₂-O-CH₂-CH₂-O

RN 705445-15-4 CAPLUS
CN β-D-Glucopyranoside, 5-(1H-indol-1-yl)-4-[[2-methyl-4-[2-(phenylmethoxy)ethoxy]phenyl]methyl]-1H-pyrazol-3-yl, 2,3,4,6-tetraacetate (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

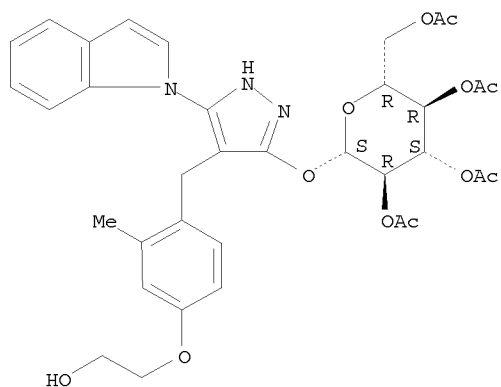
10/529,895



RN 705445-20-1 CAPLUS

CN β -D-Glucopyranoside, 4-[[4-(2-hydroxyethoxy)-2-methylphenyl]methyl]-5-(1H-indol-1-yl)-1H-pyrazol-3-yl, 2,3,4,6-tetraacetate (CA INDEX NAME)

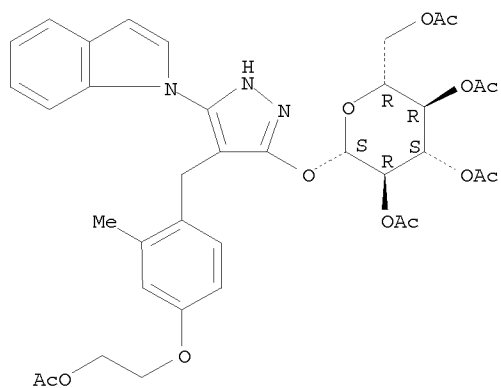
Absolute stereochemistry.



RN 705445-25-6 CAPLUS

CN β -D-Glucopyranoside, 4-[[4-[2-(acetyloxy)ethoxy]-2-methylphenyl]methyl]-5-(1H-indol-1-yl)-1H-pyrazol-3-yl, 2,3,4,6-tetraacetate (CA INDEX NAME)

Absolute stereochemistry.



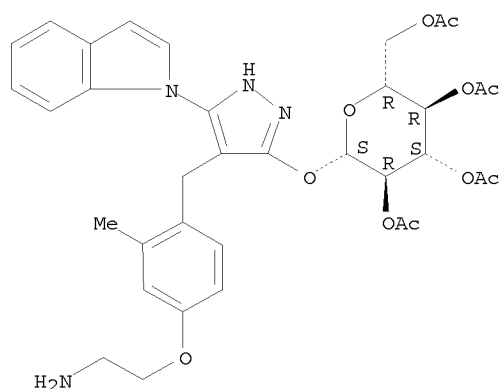
RN 705445-30-3 CAPLUS

CN β -D-Glucopyranoside, 4-[[4-(2-aminoethoxy)-2-methylphenyl]methyl]-5-(1H-indol-1-yl)-1H-pyrazol-3-yl, 2,3,4,6-tetraacetate (CA INDEX NAME)

McIntosh

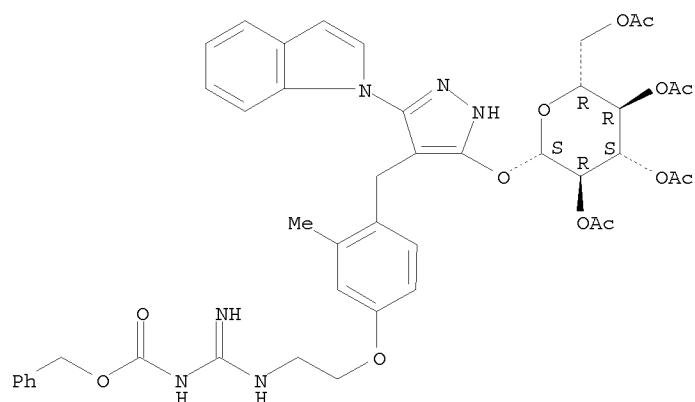
10/529,895

Absolute stereochemistry.



RN 705445-45-0 CAPLUS
CN Carbamic acid, [2-[4-[[3-(1H-indol-1-yl)-5-[(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)oxy]-1H-pyrazol-4-yl]methyl]-3-methylphenoxy]ethyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:311011 CAPLUS
DN 140:321649
TI Preparation of pyrazolyl glycoside derivatives as inhibitors of
1,5-anhydroglucitol/fructose/mannose transporters
IN Fujikura, Hideki; Kikuchi, Norihiko; Tazawa, Shigeki; Yamato, Tokuhisa;
Isaji, Masayuki
PA Kissei Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 159 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE

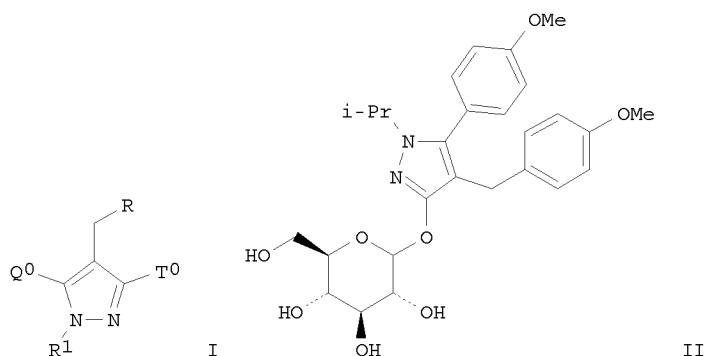
PI WO 2004031203 A1 20040415 WO 2003-JP12477 20030930
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CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,

McIntosh

PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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CA 2500873 A1 20040415 CA 2003-2500873 20030930
 AU 2003272903 A1 20040423 AU 2003-272903 20030930
 EP 1550668 A1 20050706 EP 2003-753967 20030930
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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US 20060128635 A1 20060615 US 2005-529895 20050919
 PRAI JP 2002-293090 A 20021004
 JP 2002-330694 A 20021114
 JP 2002-378959 A 20021227
 WO 2003-JP12477 W 20030930
 OS MARPAT 140:321649
 GI



AB The title compds. [I; R = each (un)substituted C3-8 cycloalkyl, C6-10 aryl, C2-9 heterocycloalkyl, or C1-9 heteroaryl; R¹ = H, each (un)substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 cycloalkyl, C6-10 aryl, C2-9 heterocycloalkyl, or C1-9 heteroaryl; one of Q⁰ and T⁰ = α - or β -D-glucopyranosyloxy or -mannopyranosyloxy or β -D-deoxyglucopyranosyloxy- and the other = (CH₂)_nAr; wherein Ar = each (un)substituted C6-10 aryl or C1-9 heteroaryl; n = an integer of 0-2] or pharmacol. acceptable salts or prodrugs thereof are prepared Also disclosed are medicinal composition containing the compound I, medicinal use thereof, and intermediates in producing the same. These compds. exerts an excellent effect of inhibiting human 1,5-anhydroglucitol/fructose/mannose transporters and inhibit reabsorption or cellular uptake of glucose, fructose, and mannose in kidney or absorption of these saccharide small intestine and inhibit the increase in blood sugar. Therefore, they are useful as preventives, progress inhibitors or remedies for a disease caused by the over intake of at least one saccharide selected from among glucose, fructose, and mannose or a disease caused by hyperglycemia (diabetic complication, diabetes, or diabetic nephropathy). Thus, glycosidation of 1-isopropyl-5-(4-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1,2-dihydro-3H-pyrazol-3-one by acetobromo- α -D-glucose in the presence of benzyltributylammonium bromide in a mixture of CH₂Cl₂ and 5 N aqueous NaOH at room temperature for 1.5 h followed by treatment of the product with NaOMe in MeOH gave 3-(β -D-glucopyranosyloxy)-1-isopropyl-5-(4-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1H-pyrazole (II). II in vitro inhibited the uptake of [14C]methyl α -D-glucopyranoside in COS-7 cells transfected with human SMINT/PME18S-FL expression plasmid with IC₅₀ of 92 nM.

IT 678993-32-3P 678993-33-4P 678993-34-5P
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10/529,895

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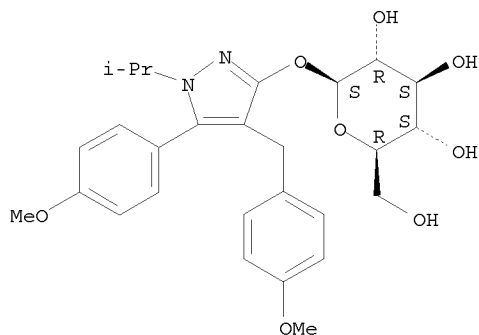
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of pyrazolyl glycoside derivs. as inhibitors of
1,5-anhydroglucitol/fructose/mannose transporters and preventives,
progress inhibitors or remedies for diabetic complication, diabetes, or
diabetic nephropathy)

RN 678993-32-3 CAPLUS

CN β -D-Glucopyranoside, 5-(4-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-
1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



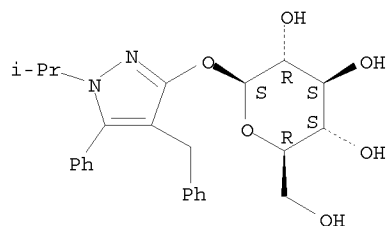
RN 678993-33-4 CAPLUS

CN β -D-Glucopyranoside, 1-(1-methylethyl)-5-phenyl-4-(phenylmethyl)-1H-
pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

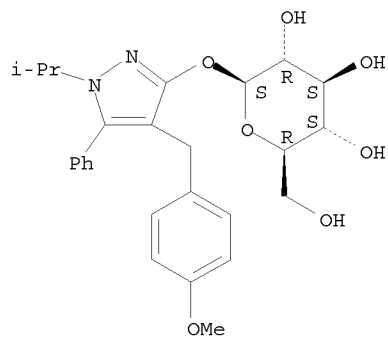
10/529,895



RN 678993-34-5 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

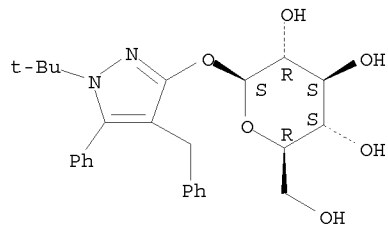
Absolute stereochemistry.



RN 678993-35-6 CAPLUS

CN β -D-Glucopyranoside, 1-(1,1-dimethylethyl)-5-phenyl-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



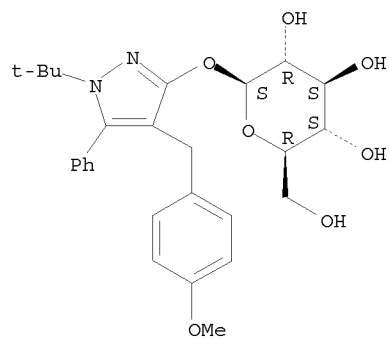
RN 678993-36-7 CAPLUS

CN β -D-Glucopyranoside, 1-(1,1-dimethylethyl)-4-[(4-methoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

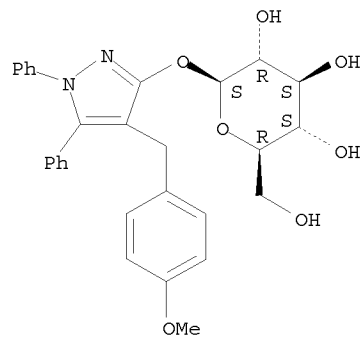
McIntosh

10/529,895



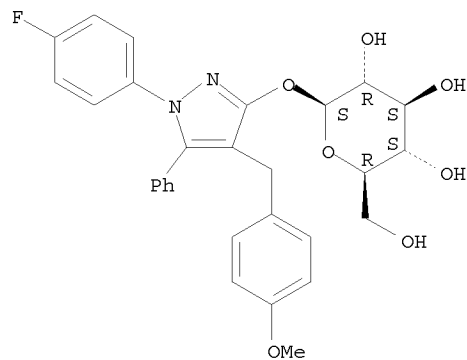
RN 678993-37-8 CAPLUS
CN β-D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1,5-diphenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



RN 678993-38-9 CAPLUS
CN β-D-Glucopyranoside, 1-(4-fluorophenyl)-4-[(4-methoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

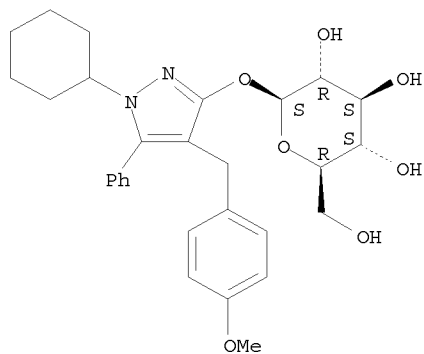


RN 678993-39-0 CAPLUS
CN β-D-Glucopyranoside, 1-cyclohexyl-4-[(4-methoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

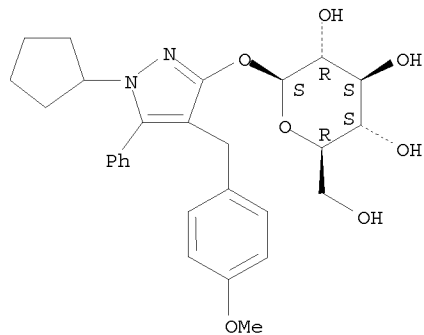
10/529,895



RN 678993-40-3 CAPLUS

CN β -D-Glucopyranoside, 1-cyclopentyl-4-[(4-methoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

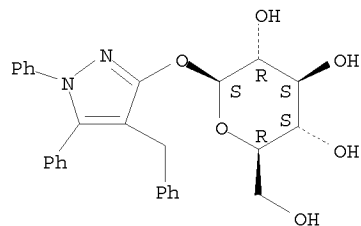
Absolute stereochemistry.



RN 678993-41-4 CAPLUS

CN β -D-Glucopyranoside, 1,5-diphenyl-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



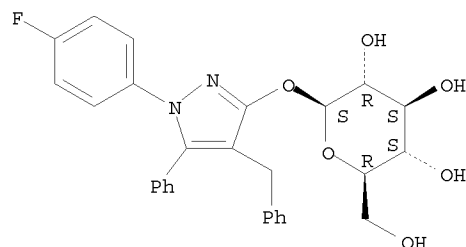
RN 678993-42-5 CAPLUS

CN β -D-Glucopyranoside, 1-(4-fluorophenyl)-5-phenyl-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

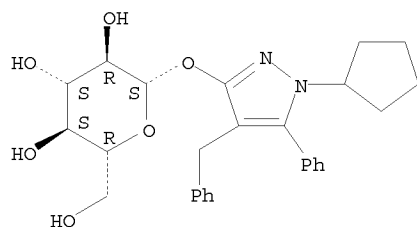
10/529,895



RN 678993-43-6 CAPLUS

CN β -D-Glucopyranoside, 1-cyclopentyl-5-phenyl-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

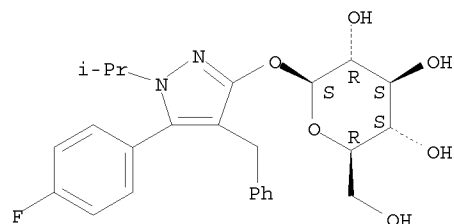
Absolute stereochemistry.



RN 678993-44-7 CAPLUS

CN β -D-Glucopyranoside, 5-(4-fluorophenyl)-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

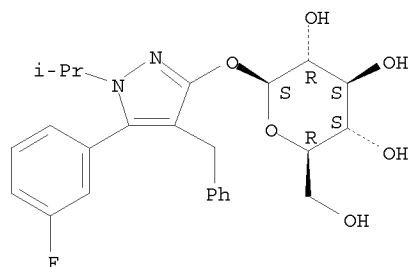
Absolute stereochemistry.



RN 678993-45-8 CAPLUS

CN β -D-Glucopyranoside, 5-(3-fluorophenyl)-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



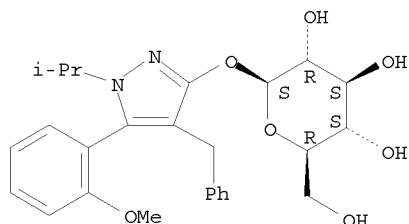
RN 678993-46-9 CAPLUS

CN β -D-Glucopyranoside, 5-(2-methoxyphenyl)-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

McIntosh

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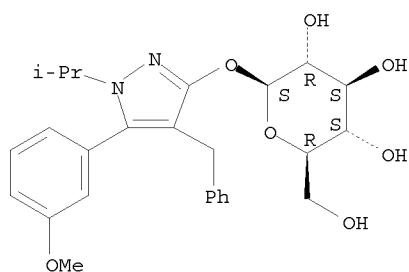
Absolute stereochemistry.



RN 678993-47-0 CAPLUS

CN β-D-Glucopyranoside, 5-(3-methoxyphenyl)-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

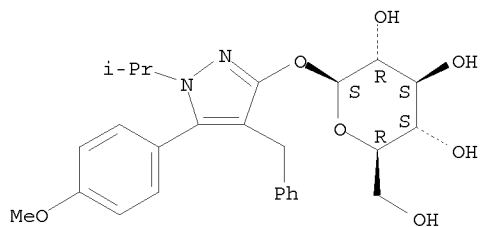
Absolute stereochemistry.



RN 678993-48-1 CAPLUS

CN β-D-Glucopyranoside, 5-(4-methoxyphenyl)-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

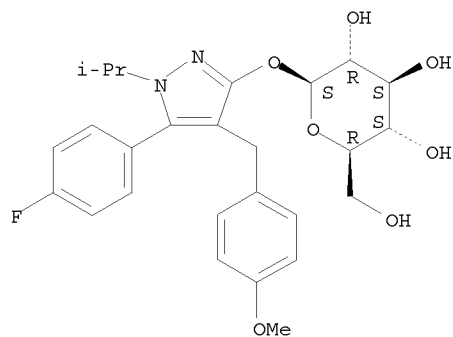
Absolute stereochemistry.



RN 678993-49-2 CAPLUS

CN β-D-Glucopyranoside, 5-(4-fluorophenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



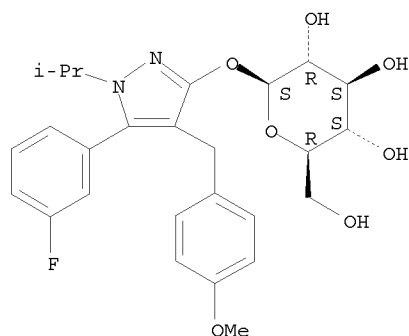
McIntosh

10/529,895

RN 678993-50-5 CAPLUS

CN β -D-Glucopyranoside, 5-(3-fluorophenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

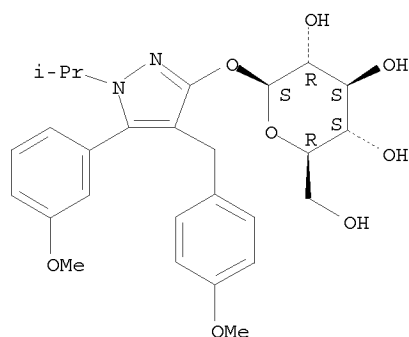
Absolute stereochemistry.



RN 678993-51-6 CAPLUS

CN β -D-Glucopyranoside, 5-(3-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

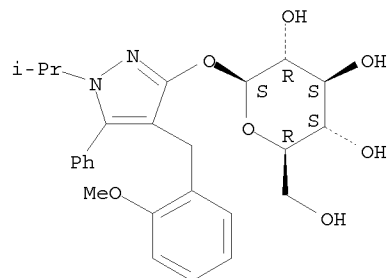
Absolute stereochemistry.



RN 678993-52-7 CAPLUS

CN β -D-Glucopyranoside, 4-[(2-methoxyphenyl)methyl]-1-(1-methylethyl)-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



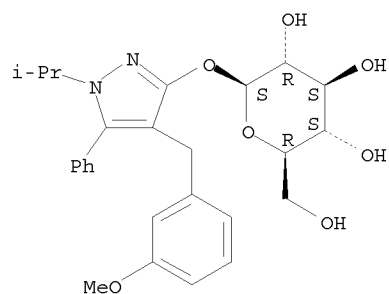
RN 678993-53-8 CAPLUS

CN β -D-Glucopyranoside, 4-[(3-methoxyphenyl)methyl]-1-(1-methylethyl)-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

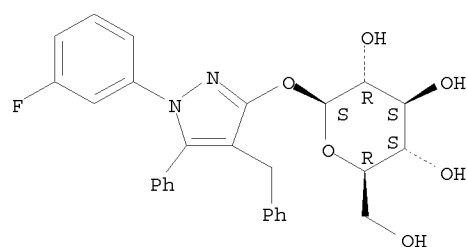
10/529,895



RN 678993-54-9 CAPLUS

CN β -D-Glucopyranoside, 1-(3-fluorophenyl)-5-phenyl-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

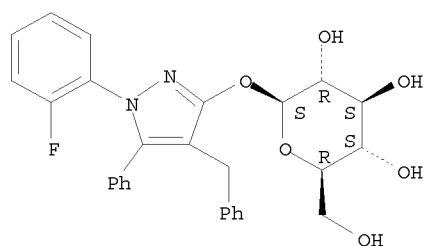
Absolute stereochemistry.



RN 678993-55-0 CAPLUS

CN β -D-Glucopyranoside, 1-(2-fluorophenyl)-5-phenyl-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

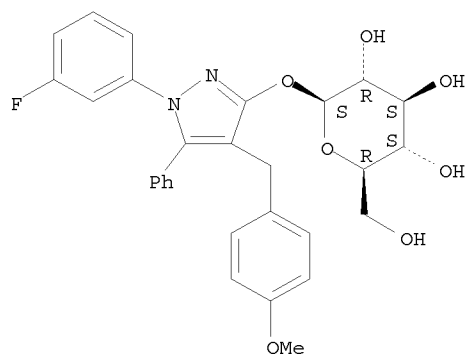


RN 678993-56-1 CAPLUS

CN β -D-Glucopyranoside, 1-(3-fluorophenyl)-4-[(4-methoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

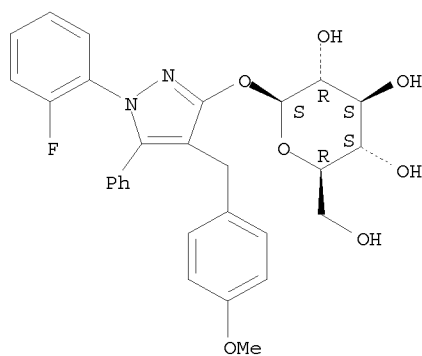
10/529,895



RN 678993-57-2 CAPLUS

CN β-D-Glucopyranoside, 1-(2-fluorophenyl)-4-[(4-methoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

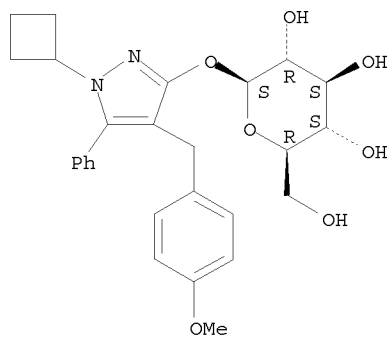
Absolute stereochemistry.



RN 678993-58-3 CAPLUS

CN β-D-Glucopyranoside, 1-cyclobutyl-4-[(4-methoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



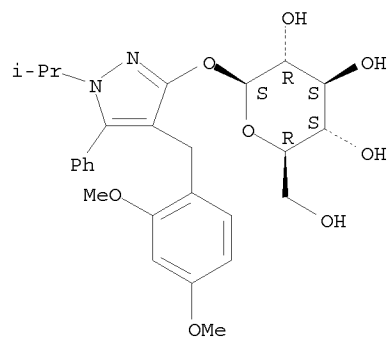
RN 678993-59-4 CAPLUS

CN β-D-Glucopyranoside, 4-[(2,4-dimethoxyphenyl)methyl]-1-(1-methylethyl)-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

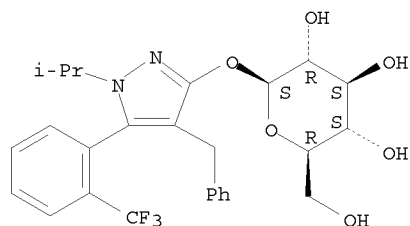
10/529,895



RN 678993-60-7 CAPLUS

CN β-D-Glucopyranoside, 1-(1-methylethyl)-4-(phenylmethyl)-5-[2-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

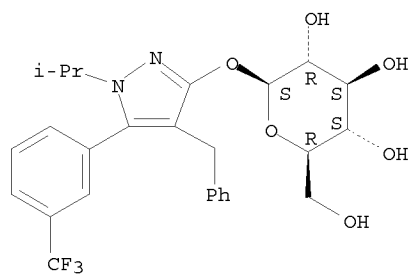
Absolute stereochemistry.



RN 678993-61-8 CAPLUS

CN β-D-Glucopyranoside, 1-(1-methylethyl)-4-(phenylmethyl)-5-[3-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

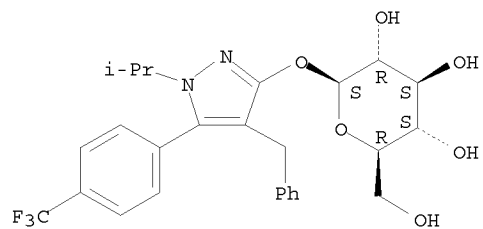
Absolute stereochemistry.



RN 678993-62-9 CAPLUS

CN β-D-Glucopyranoside, 1-(1-methylethyl)-4-(phenylmethyl)-5-[4-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



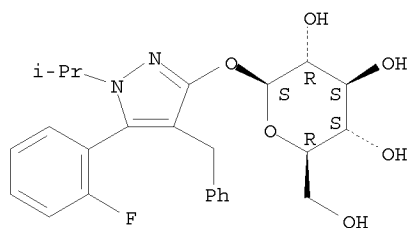
McIntosh

10/529,895

RN 678993-63-0 CAPLUS

CN β -D-Glucopyranoside, 5-(2-fluorophenyl)-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

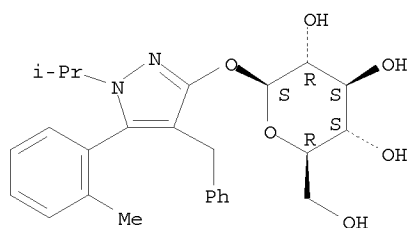
Absolute stereochemistry.



RN 678993-64-1 CAPLUS

CN β -D-Glucopyranoside, 1-(1-methylethyl)-5-(2-methylphenyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

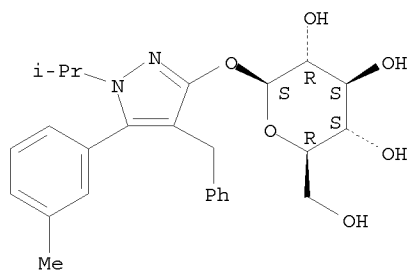
Absolute stereochemistry.



RN 678993-65-2 CAPLUS

CN β -D-Glucopyranoside, 1-(1-methylethyl)-5-(3-methylphenyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

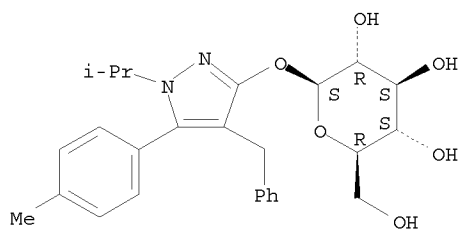
Absolute stereochemistry.



RN 678993-66-3 CAPLUS

CN β -D-Glucopyranoside, 1-(1-methylethyl)-5-(4-methylphenyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



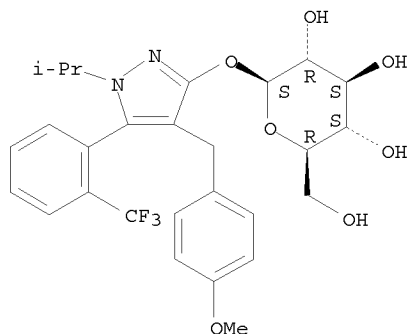
McIntosh

10/529,895

RN 678993-67-4 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-[2-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

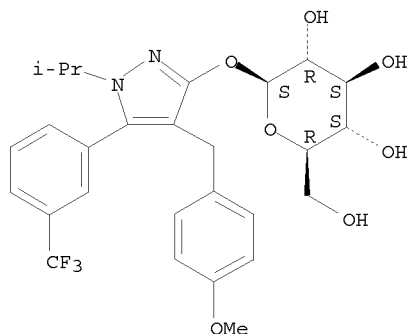
Absolute stereochemistry.



RN 678993-68-5 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-[3-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

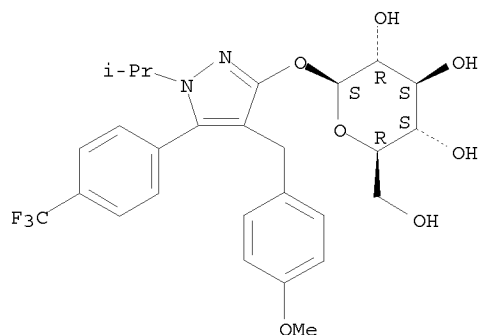
Absolute stereochemistry.



RN 678993-69-6 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-[4-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



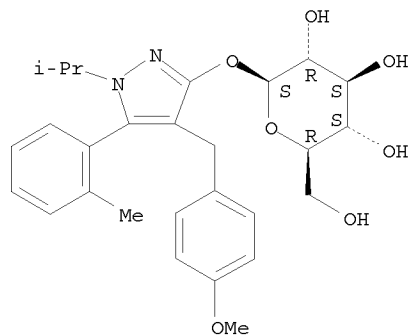
RN 678993-70-9 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-(2-methylphenyl)-1H-pyrazol-3-yl (CA INDEX NAME)

McIntosh

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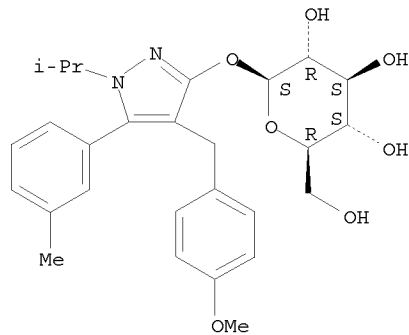
Absolute stereochemistry.



RN 678993-71-0 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-(3-methylphenyl)-1H-pyrazol-3-yl (CA INDEX NAME)

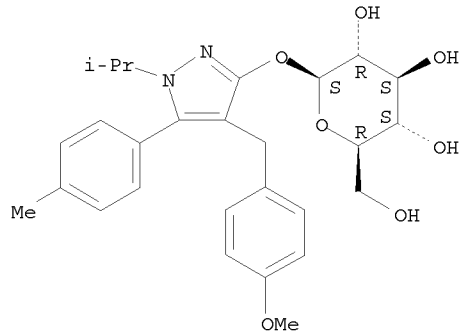
Absolute stereochemistry.



RN 678993-72-1 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-(4-methylphenyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



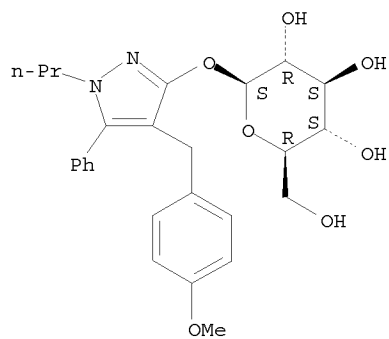
RN 678993-73-2 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-5-phenyl-1-propyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

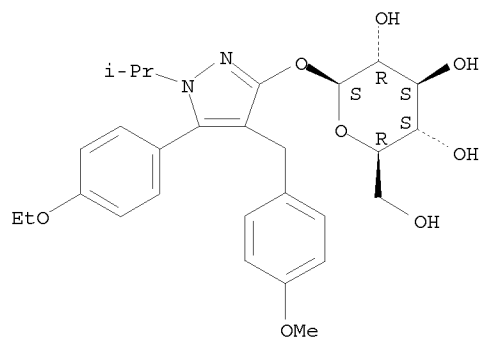
10/529,895



RN 678993-74-3 CAPLUS

CN β -D-Glucopyranoside, 5-(4-ethoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

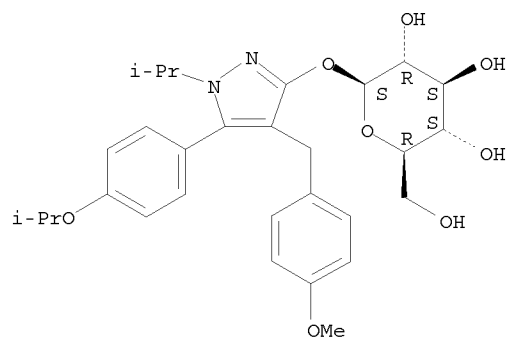
Absolute stereochemistry.



RN 678993-75-4 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-5-[4-(1-methylethoxy)phenyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



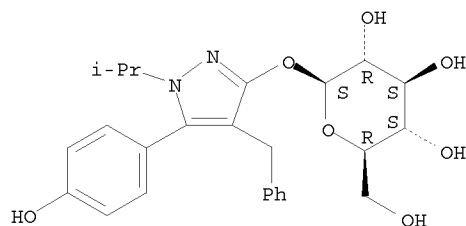
RN 678993-76-5 CAPLUS

CN β -D-Glucopyranoside, 5-(4-hydroxyphenyl)-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

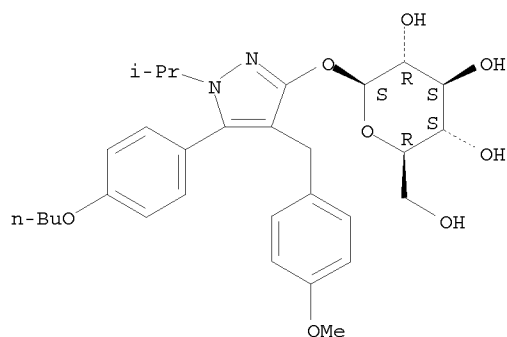
10/529,895



RN 678993-77-6 CAPLUS

CN β -D-Glucopyranoside, 5-(4-butoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

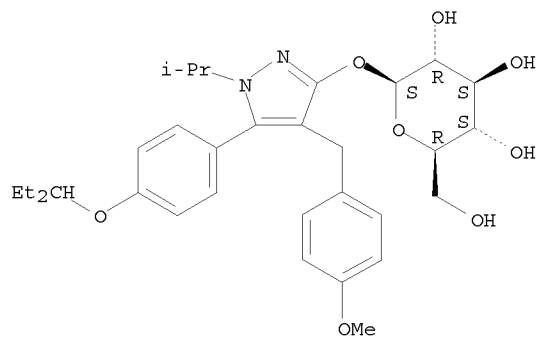
Absolute stereochemistry.



RN 678993-78-7 CAPLUS

CN β -D-Glucopyranoside, 5-[4-(1-ethylpropoxy)phenyl]-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



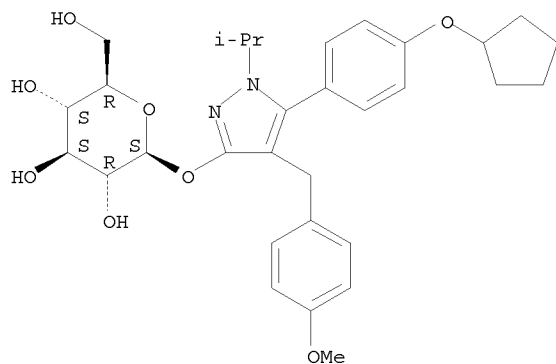
RN 678993-79-8 CAPLUS

CN β -D-Glucopyranoside, 5-[4-(cyclopentyloxy)phenyl]-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

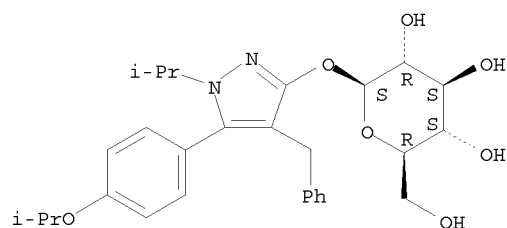
10/529,895



RN 678993-80-1 CAPLUS

CN β -D-Glucopyranoside, 5-[4-(1-methylethoxy)phenyl]-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

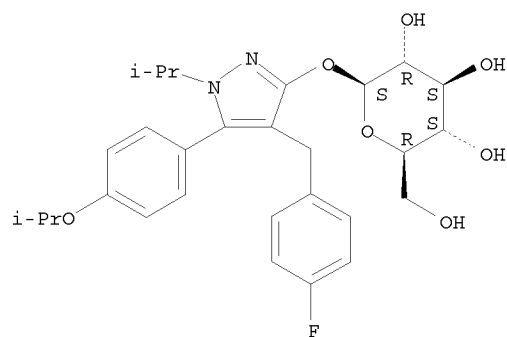
Absolute stereochemistry.



RN 678993-81-2 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-fluorophenyl)methyl]-5-[4-(1-methylethoxy)phenyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



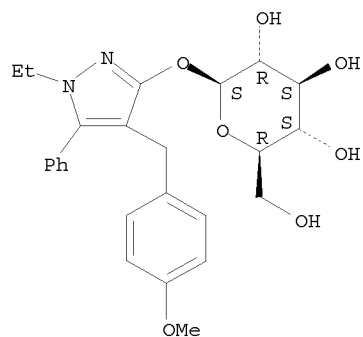
RN 678993-82-3 CAPLUS

CN β -D-Glucopyranoside, 1-ethyl-4-[(4-methoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

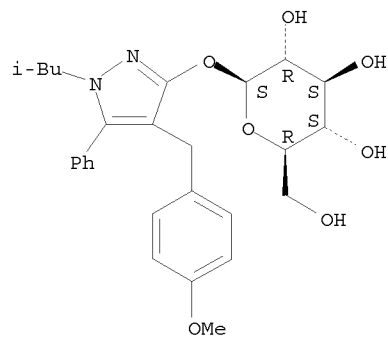
10/529,895



RN 678993-83-4 CAPLUS

CN β-D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(2-methylpropyl)-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

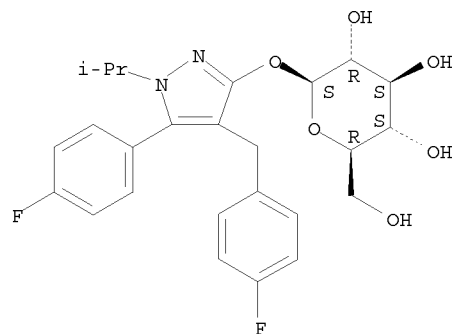
Absolute stereochemistry.



RN 678993-84-5 CAPLUS

CN β-D-Glucopyranoside, 5-(4-fluorophenyl)-4-[(4-fluorophenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



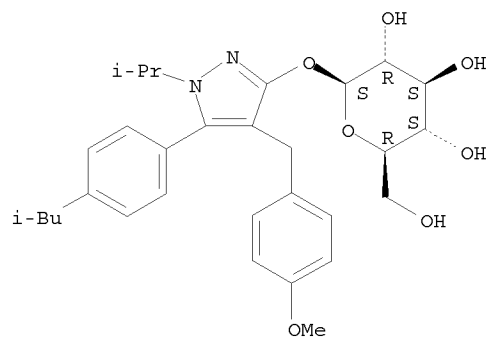
RN 678993-85-6 CAPLUS

CN β-D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-[4-(2-methylpropyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

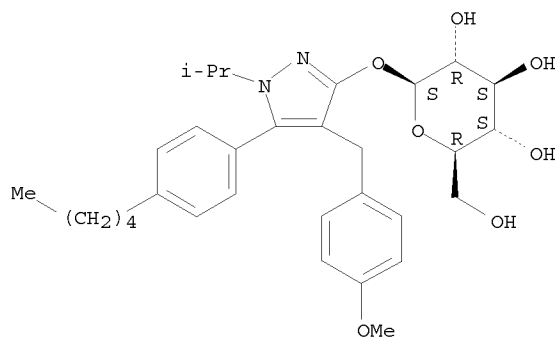
10/529,895



RN 678993-86-7 CAPLUS

CN β-D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-(4-pentylphenyl)-1H-pyrazol-3-yl (CA INDEX NAME)

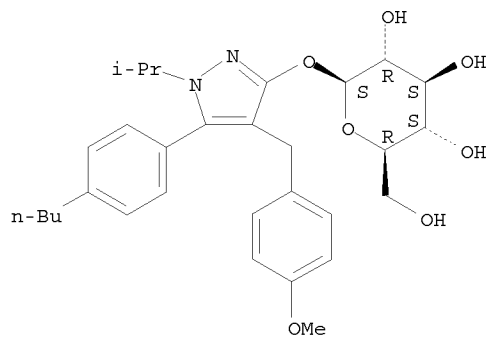
Absolute stereochemistry.



RN 678993-87-8 CAPLUS

CN β-D-Glucopyranoside, 5-(4-butylphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



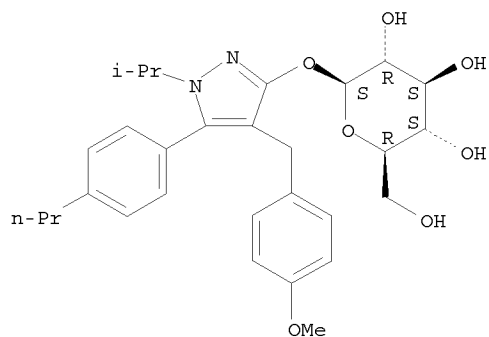
RN 678993-88-9 CAPLUS

CN β-D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-(4-propylphenyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

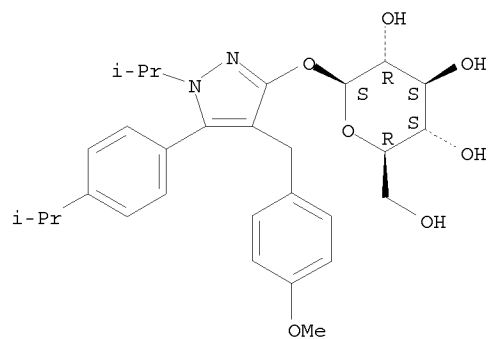
10/529,895



RN 678993-89-0 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-[4-(1-methylethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

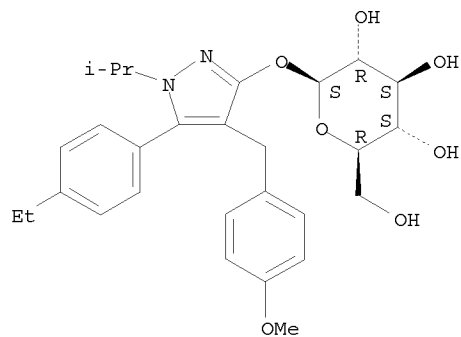
Absolute stereochemistry.



RN 678993-90-3 CAPLUS

CN β -D-Glucopyranoside, 5-(4-ethylphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



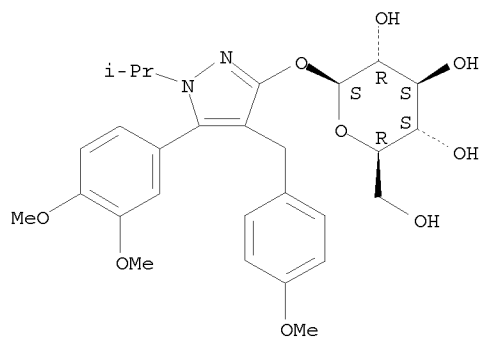
RN 678993-91-4 CAPLUS

CN β -D-Glucopyranoside, 5-(3,4-dimethoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

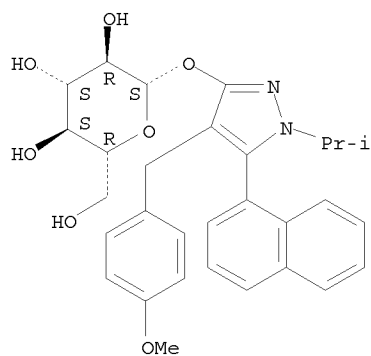
10/529,895



RN 678993-92-5 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-(1-naphthalenyl)-1H-pyrazol-3-yl (CA INDEX NAME)

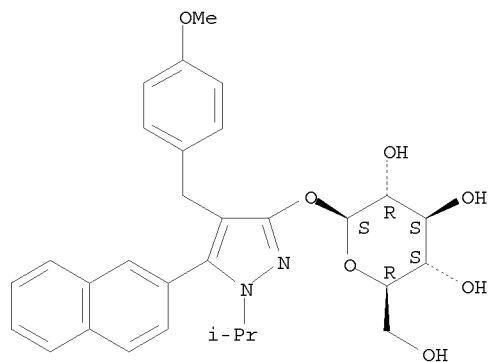
Absolute stereochemistry.



RN 678993-93-6 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-(2-naphthalenyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



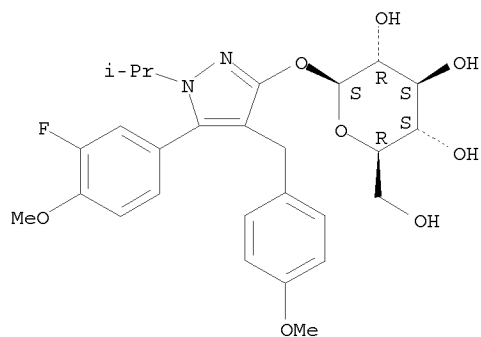
RN 678993-94-7 CAPLUS

CN β -D-Glucopyranoside, 5-(3-fluoro-4-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

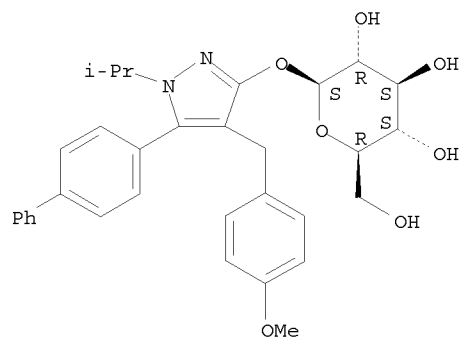
10/529,895



RN 678993-95-8 CAPLUS

CN β -D-Glucopyranoside, 5-[1,1'-biphenyl]-4-yl-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

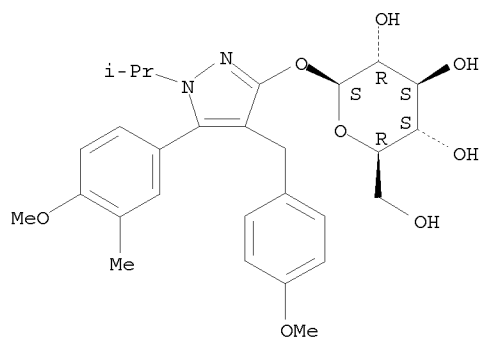
Absolute stereochemistry.



RN 678993-96-9 CAPLUS

CN β -D-Glucopyranoside, 5-(4-methoxy-3-methylphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



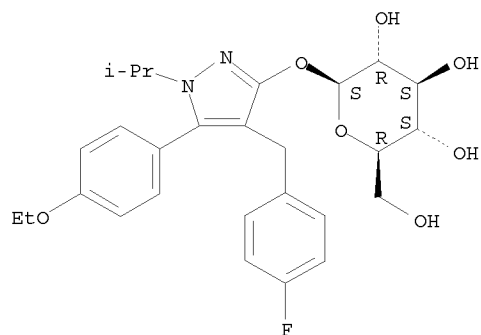
RN 678993-97-0 CAPLUS

CN β -D-Glucopyranoside, 5-(4-ethoxyphenyl)-4-[(4-fluorophenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

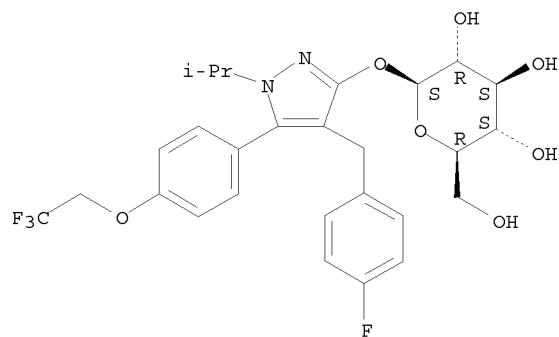
10/529,895



RN 678993-98-1 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-fluorophenyl)methyl]-1-(1-methylethyl)-5-[4-(2,2,2-trifluoroethoxy)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

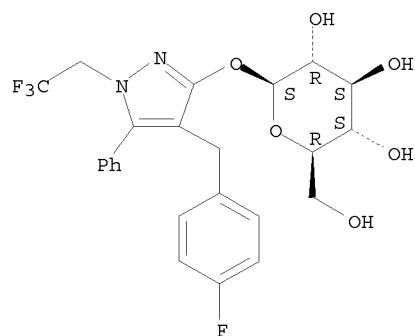
Absolute stereochemistry.



RN 678993-99-2 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-fluorophenyl)methyl]-5-phenyl-1-(2,2,2-trifluoroethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



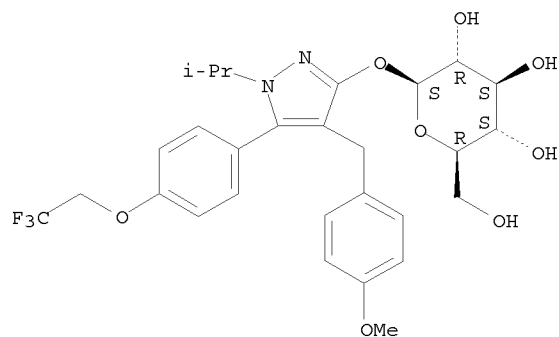
RN 678994-00-8 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-[4-(2,2,2-trifluoroethoxy)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

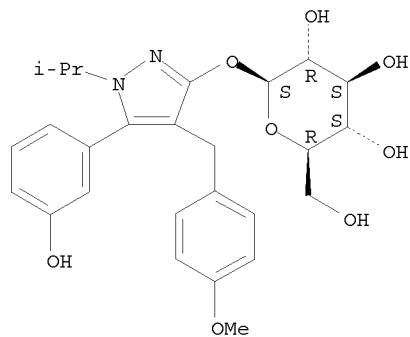
10/529,895



RN 678994-01-9 CAPLUS

CN β-D-Glucopyranoside, 5-(3-hydroxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

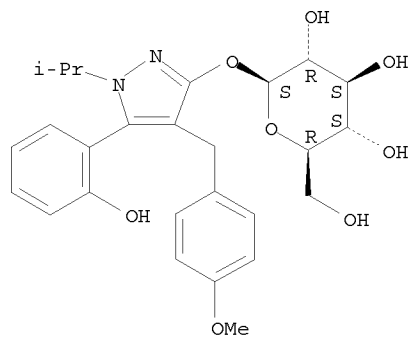
Absolute stereochemistry.



RN 678994-02-0 CAPLUS

CN β-D-Glucopyranoside, 5-(2-hydroxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



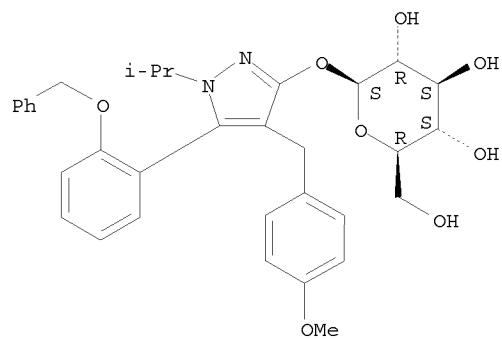
RN 678994-03-1 CAPLUS

CN β-D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-[2-(phenylmethoxy)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

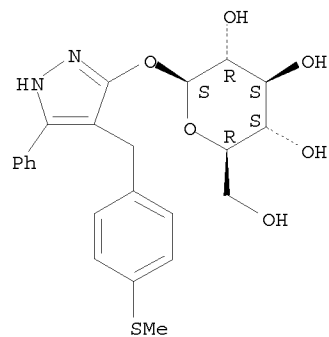
10/529,895



RN 678994-04-2 CAPLUS

CN β-D-Glucopyranoside, 4-[[4-(methylthio)phenyl]methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

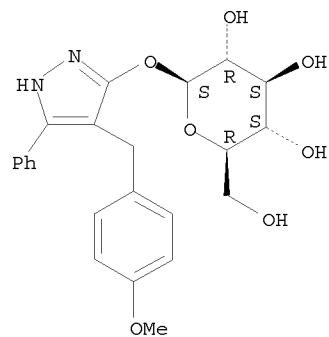
Absolute stereochemistry.



RN 678994-05-3 CAPLUS

CN β-D-Glucopyranoside, 4-[[4-methoxyphenyl]methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



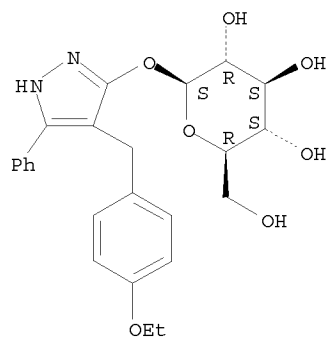
RN 678994-06-4 CAPLUS

CN β-D-Glucopyranoside, 4-[[4-ethoxyphenyl]methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

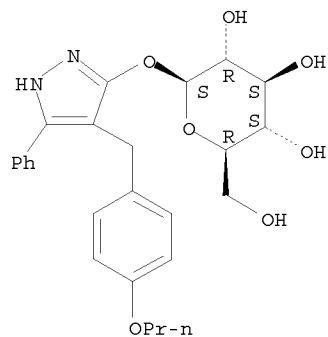
10/529,895



RN 678994-07-5 CAPLUS

CN β-D-Glucopyranoside, 5-phenyl-4-[(4-propoxyphenyl)methyl]-1H-pyrazol-3-yl (CA INDEX NAME)

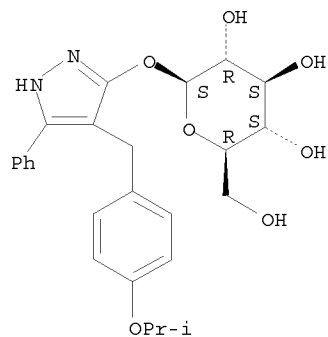
Absolute stereochemistry.



RN 678994-08-6 CAPLUS

CN β-D-Glucopyranoside, 4-[[4-(1-methylethoxy)phenyl]methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



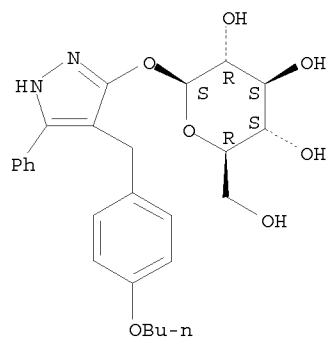
RN 678994-09-7 CAPLUS

CN β-D-Glucopyranoside, 4-[(4-butoxyphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

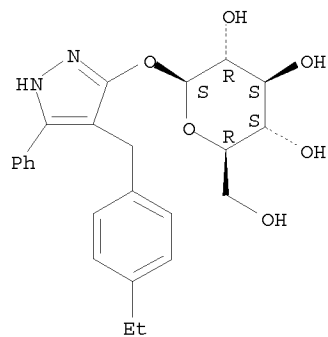
10/529,895



RN 678994-10-0 CAPLUS

CN β-D-Glucopyranoside, 4-[(4-ethylphenyl)methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

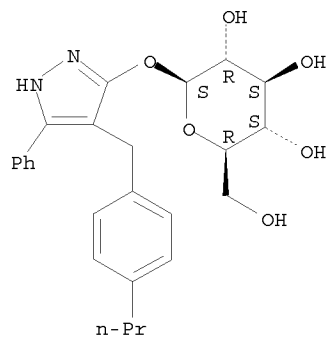
Absolute stereochemistry.



RN 678994-11-1 CAPLUS

CN β-D-Glucopyranoside, 5-phenyl-4-[(4-propylphenyl)methyl]-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



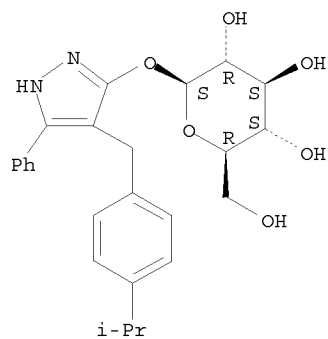
RN 678994-12-2 CAPLUS

CN β-D-Glucopyranoside, 4-[[4-(1-methylethyl)phenyl]methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

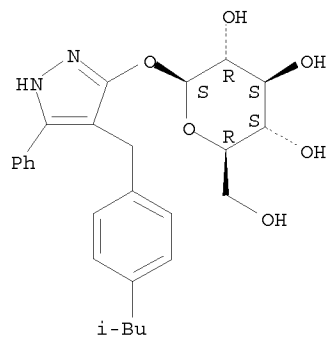
10/529,895



RN 678994-13-3 CAPLUS

CN β -D-Glucopyranoside, 4-[[4-(2-methylpropyl)phenyl]methyl]-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

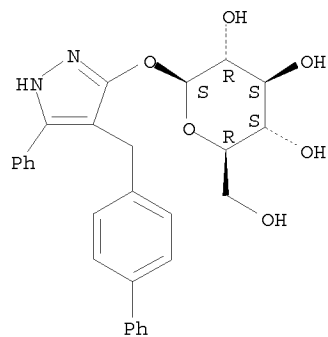
Absolute stereochemistry.



RN 678994-14-4 CAPLUS

CN β -D-Glucopyranoside, 4-([1,1'-biphenyl]-4-ylmethyl)-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



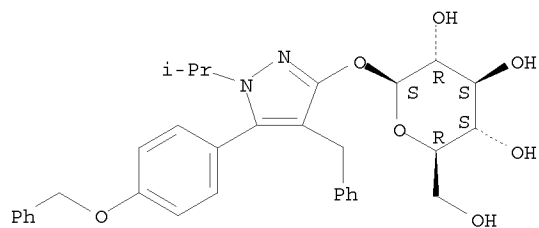
RN 678994-15-5 CAPLUS

CN β -D-Glucopyranoside, 1-(1-methylethyl)-5-[4-(phenylmethoxy)phenyl]-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

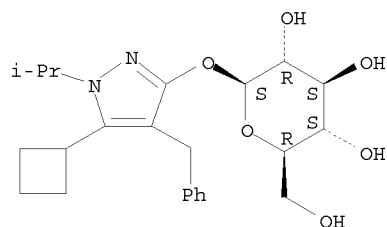
10/529,895



RN 678994-23-5 CAPLUS

CN β -D-Glucopyranoside, 5-cyclobutyl-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

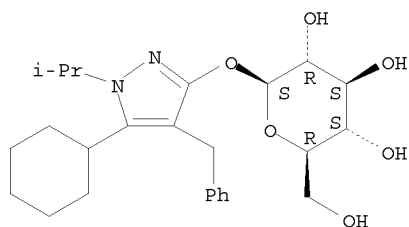
Absolute stereochemistry.



RN 678994-24-6 CAPLUS

CN β -D-Glucopyranoside, 5-cyclohexyl-1-(1-methylethyl)-4-(phenylmethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

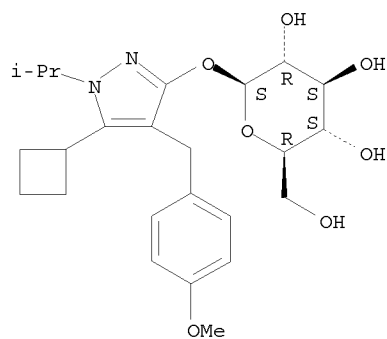
Absolute stereochemistry.



RN 678994-25-7 CAPLUS

CN β -D-Glucopyranoside, 5-cyclobutyl-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



RN 678994-26-8 CAPLUS

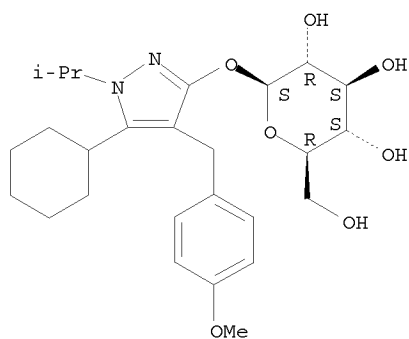
CN β -D-Glucopyranoside, 5-cyclohexyl-4-[(4-methoxyphenyl)methyl]-1-(1-

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methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

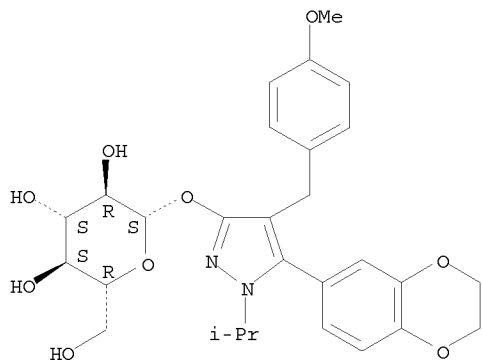
Absolute stereochemistry.



RN 678994-48-4 CAPLUS

CN β -D-Glucopyranoside, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

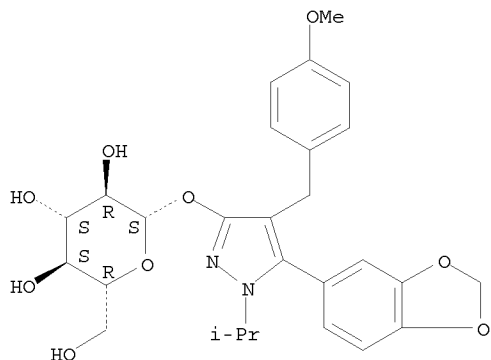
Absolute stereochemistry.



RN 678994-49-5 CAPLUS

CN β -D-Glucopyranoside, 5-(1,3-benzodioxol-5-yl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



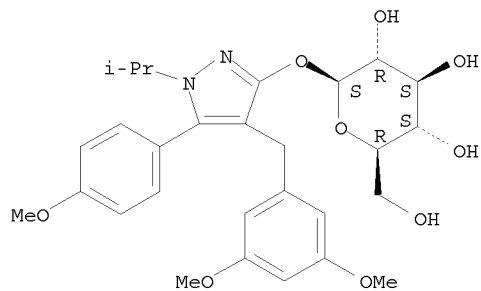
RN 678994-50-8 CAPLUS

CN β -D-Glucopyranoside, 4-[(3,5-dimethoxyphenyl)methyl]-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

McIntosh

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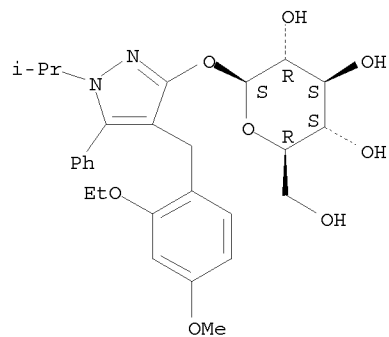
Absolute stereochemistry.



RN 678994-51-9 CAPLUS

CN β-D-Glucopyranoside, 4-[(2-ethoxy-4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

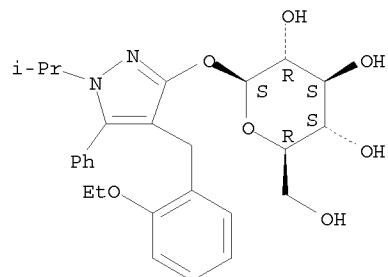
Absolute stereochemistry.



RN 678994-52-0 CAPLUS

CN β-D-Glucopyranoside, 4-[(2-ethoxyphenyl)methyl]-1-(1-methylethyl)-5-phenyl-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



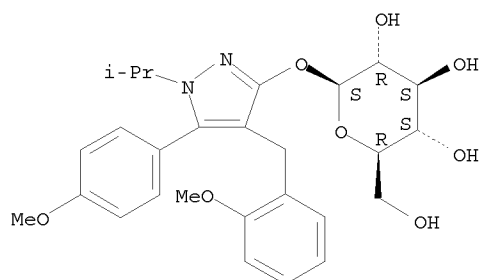
RN 678994-53-1 CAPLUS

CN β-D-Glucopyranoside, 5-(4-methoxyphenyl)-4-[(2-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

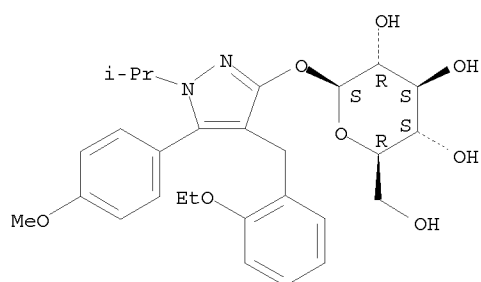
10/529,895



RN 678994-54-2 CAPLUS

CN β -D-Glucopyranoside, 4-[(2-ethoxyphenyl)methyl]-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

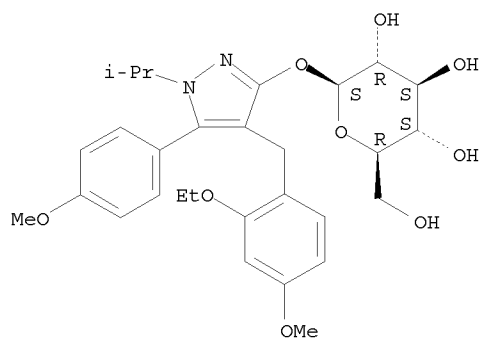
Absolute stereochemistry.



RN 678994-55-3 CAPLUS

CN β -D-Glucopyranoside, 4-[(2-ethoxy-4-methoxyphenyl)methyl]-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



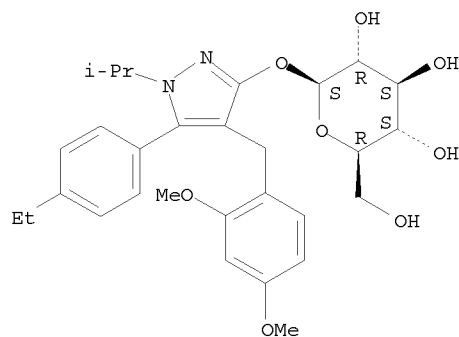
RN 678994-56-4 CAPLUS

CN β -D-Glucopyranoside, 4-[(2,4-dimethoxyphenyl)methyl]-5-(4-ethylphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

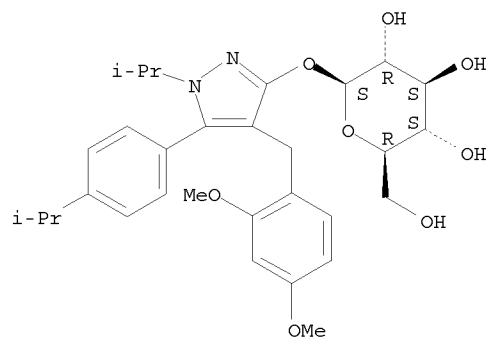
10/529,895



RN 678994-57-5 CAPLUS

CN β -D-Glucopyranoside, 4-[(2,4-dimethoxyphenyl)methyl]-1-(1-methylethyl)-5-[4-(1-methylethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

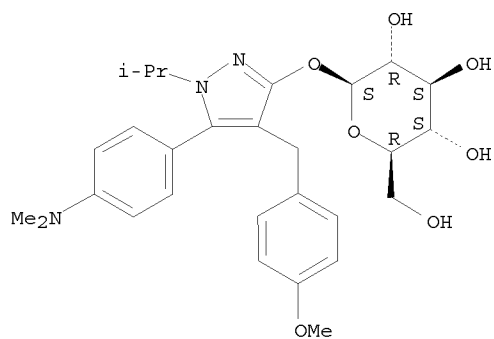
Absolute stereochemistry.



RN 678994-58-6 CAPLUS

CN β -D-Glucopyranoside, 5-[4-(dimethylamino)phenyl]-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



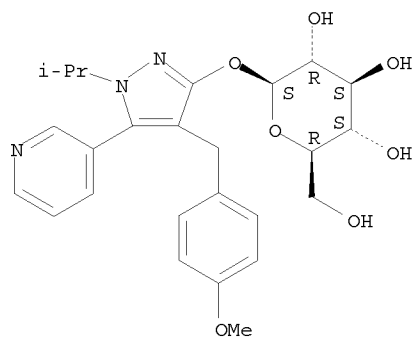
RN 678994-59-7 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-5-(3-pyridinyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

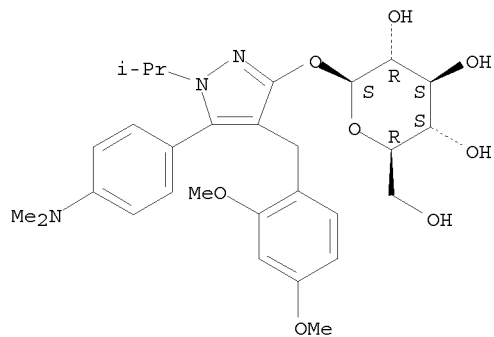
10/529,895



RN 678994-60-0 CAPLUS

CN β-D-Glucopyranoside, 4-[(2,4-dimethoxyphenyl)methyl]-5-[4-(dimethylamino)phenyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

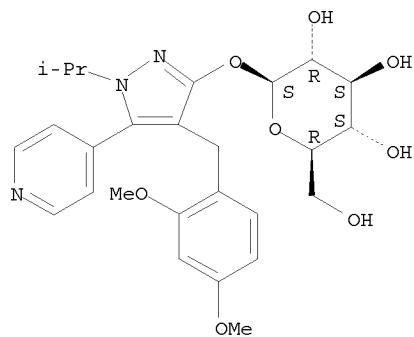
Absolute stereochemistry.



RN 678994-61-1 CAPLUS

CN β-D-Glucopyranoside, 4-[(2,4-dimethoxyphenyl)methyl]-1-(1-methylethyl)-5-(4-pyridinyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



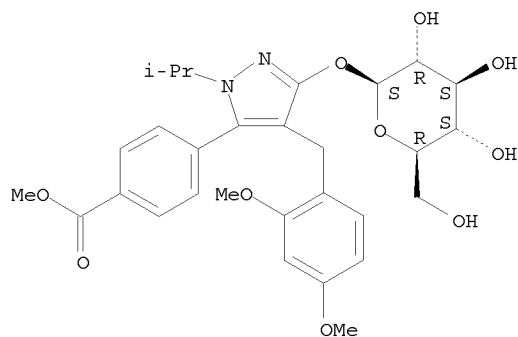
RN 678994-62-2 CAPLUS

CN Benzoic acid, 4-[4-[(2,4-dimethoxyphenyl)methyl]-3-(β-D-glucopyranosyloxy)-1-(1-methylethyl)-1H-pyrazol-5-yl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

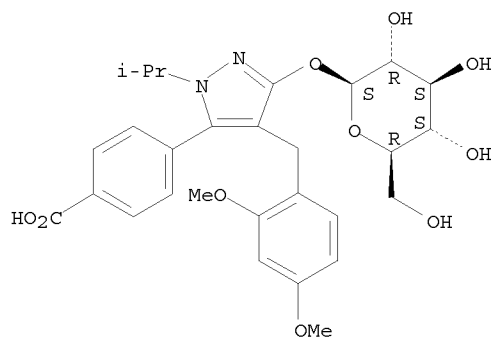
10/529,895



RN 678994-63-3 CAPLUS

CN Benzoic acid, 4-[4-[(2,4-dimethoxyphenyl)methyl]-3-(β-D-glucopyranosyloxy)-1-(1-methylethyl)-1H-pyrazol-5-yl]- (CA INDEX NAME)

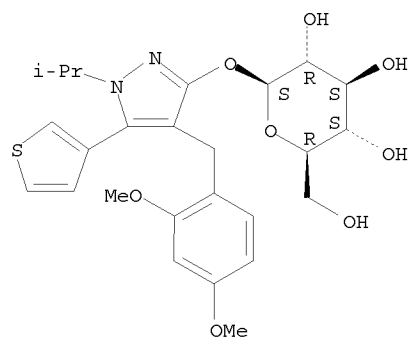
Absolute stereochemistry.



RN 678994-64-4 CAPLUS

CN β-D-Glucopyranoside, 4-[(2,4-dimethoxyphenyl)methyl]-1-(1-methylethyl)-5-(3-thienyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



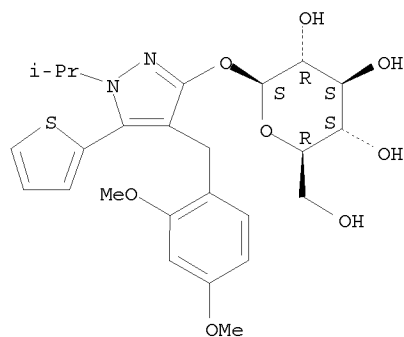
RN 678994-65-5 CAPLUS

CN β-D-Glucopyranoside, 4-[(2,4-dimethoxyphenyl)methyl]-1-(1-methylethyl)-5-(2-thienyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

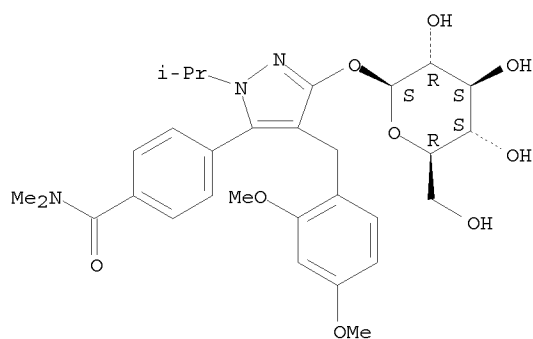
10/529,895



RN 678994-66-6 CAPLUS

CN Benzamide, 4-[4-[(2,4-dimethoxyphenyl)methyl]-3-(β-D-glucopyranosyloxy)-1-(1-methylethyl)-1H-pyrazol-5-yl]-N,N-dimethyl- (CA INDEX NAME)

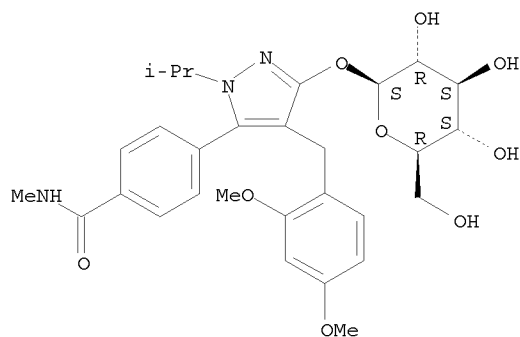
Absolute stereochemistry.



RN 678994-67-7 CAPLUS

CN Benzamide, 4-[4-[(2,4-dimethoxyphenyl)methyl]-3-(β-D-glucopyranosyloxy)-1-(1-methylethyl)-1H-pyrazol-5-yl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



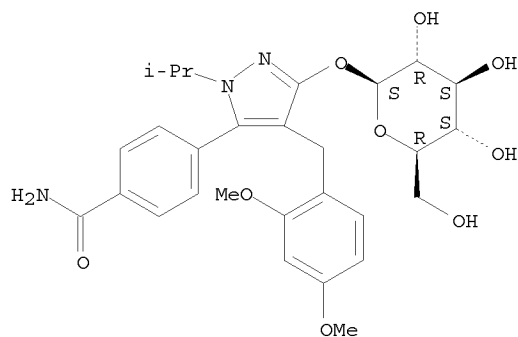
RN 678994-68-8 CAPLUS

CN Benzamide, 4-[4-[(2,4-dimethoxyphenyl)methyl]-3-(β-D-glucopyranosyloxy)-1-(1-methylethyl)-1H-pyrazol-5-yl]- (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

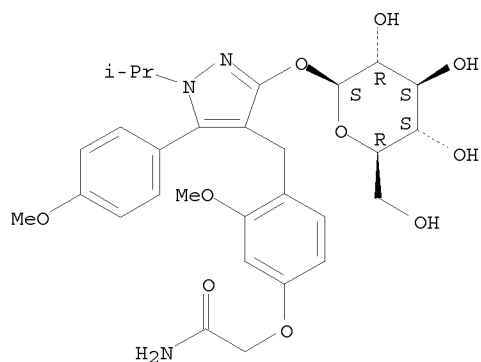
10/529,895



RN 678994-69-9 CAPLUS

CN Acetamide, 2-[4-[[3-(β -D-glucopyranosyloxy)-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-3-methoxyphenoxy]- (CA INDEX NAME)

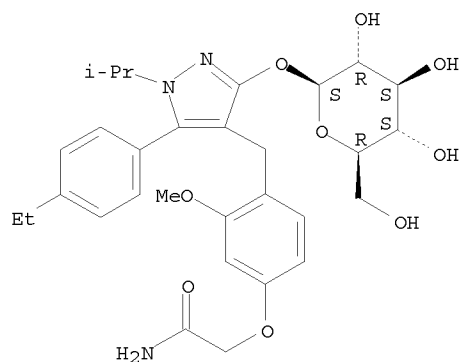
Absolute stereochemistry.



RN 678994-70-2 CAPLUS

CN Acetamide, 2-[4-[[5-(4-ethylphenyl)-3-(β -D-glucopyranosyloxy)-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-3-methoxyphenoxy]- (CA INDEX NAME)

Absolute stereochemistry.



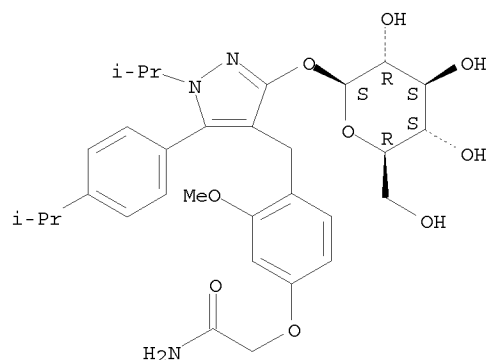
RN 678994-71-3 CAPLUS

CN Acetamide, 2-[4-[[3-(β -D-glucopyranosyloxy)-1-(1-methylethyl)-5-[4-(1-methylethyl)phenyl]-1H-pyrazol-4-yl]methyl]-3-methoxyphenoxy]- (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

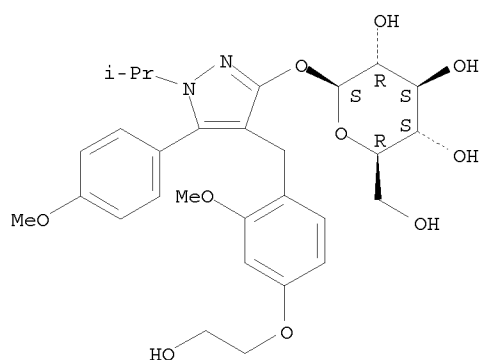
10/529,895



RN 678994-72-4 CAPLUS

CN β -D-Glucopyranoside, 4-[[4-(2-hydroxyethoxy)-2-methoxyphenyl]methyl]-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

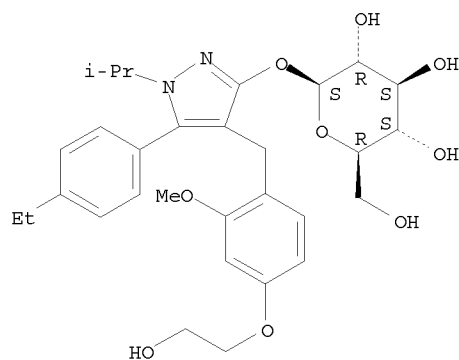
Absolute stereochemistry.



RN 678994-73-5 CAPLUS

CN β -D-Glucopyranoside, 5-(4-ethylphenyl)-4-[[4-(2-hydroxyethoxy)-2-methoxyphenyl]methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



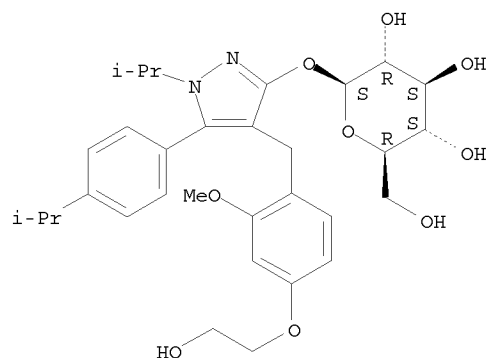
RN 678994-74-6 CAPLUS

CN β -D-Glucopyranoside, 4-[[4-(2-hydroxyethoxy)-2-methoxyphenyl]methyl]-1-(1-methylethyl)-5-[4-(1-methylethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

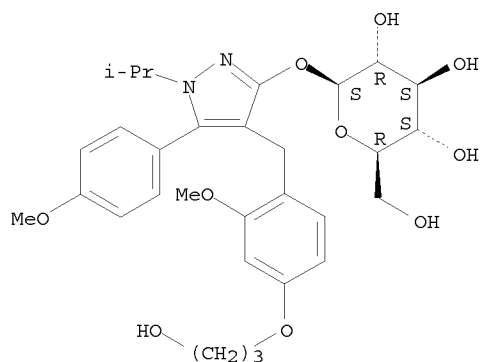
McIntosh

10/529,895



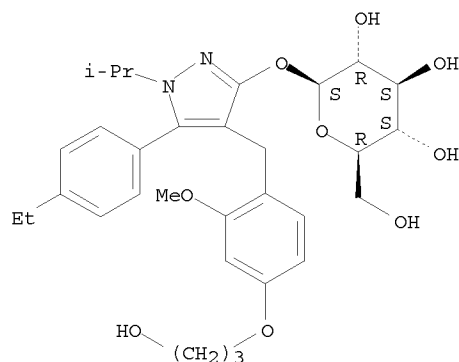
RN 678994-75-7 CAPLUS
CN β -D-Glucopyranoside, 4-[[4-(3-hydroxypropoxy)-2-methoxyphenyl]methyl]-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



RN 678994-76-8 CAPLUS
CN β -D-Glucopyranoside, 5-(4-ethylphenyl)-4-[[4-(3-hydroxypropoxy)-2-methoxyphenyl]methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

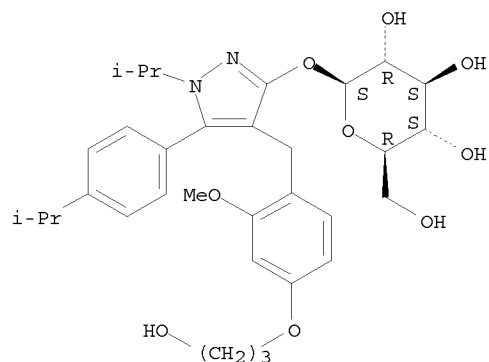


RN 678994-77-9 CAPLUS
CN β -D-Glucopyranoside, 4-[[4-(3-hydroxypropoxy)-2-methoxyphenyl]methyl]-1-(1-methylethyl)-5-[4-(1-methylethyl)phenyl]-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

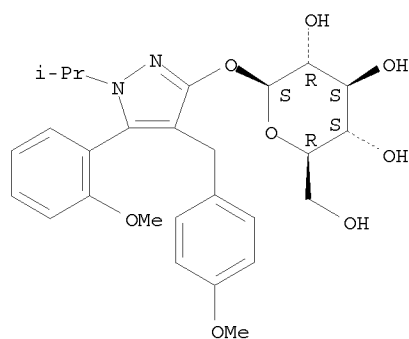
10/529,895



RN 679392-47-3 CAPLUS

CN β -D-Glucopyranoside, 5-(2-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

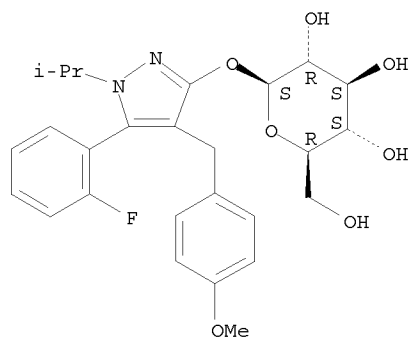
Absolute stereochemistry.



RN 679392-48-4 CAPLUS

CN β -D-Glucopyranoside, 5-(2-fluorophenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.



IT 678994-82-6P 678994-83-7P 678994-84-8P
678994-95-1P 678994-96-2P 678994-98-4P
678995-00-1P 678995-09-0P 678995-10-3P
678995-13-6P 678995-14-7P 678995-15-8P
678995-16-9P 678995-17-0P 678995-18-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrazolyl glycoside derivs. as inhibitors of 1,5-anhydroglucitol/fructose/mannose transporters and preventives,

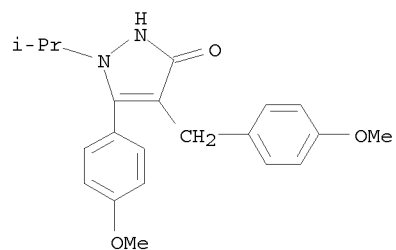
McIntosh

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progress inhibitors or remedies for diabetic complication, diabetes, or diabetic nephropathy)

RN 678994-82-6 CAPLUS

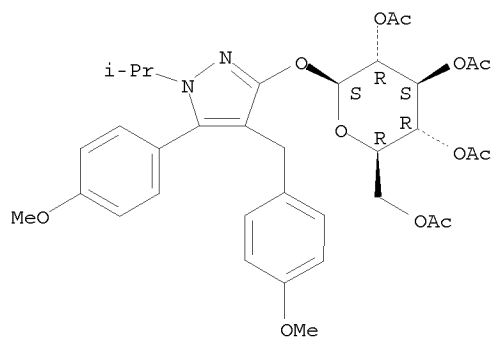
CN 3H-Pyrazol-3-one, 1,2-dihydro-5-(4-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)- (CA INDEX NAME)



RN 678994-83-7 CAPLUS

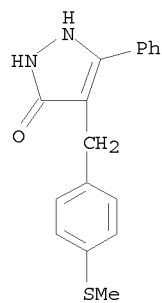
CN β -D-Glucopyranoside, 5-(4-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl, 2,3,4,6-tetraacetate (CA INDEX NAME)

Absolute stereochemistry.



RN 678994-84-8 CAPLUS

CN 3H-Pyrazol-3-one, 1,2-dihydro-4-[[4-(methylthio)phenyl]methyl]-5-phenyl- (CA INDEX NAME)

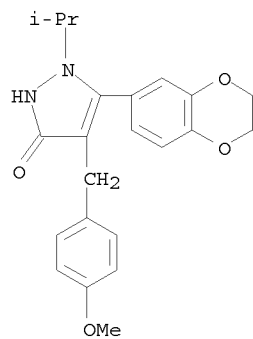


RN 678994-95-1 CAPLUS

CN 3H-Pyrazol-3-one, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-1,2-dihydro-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)- (CA INDEX NAME)

McIntosh

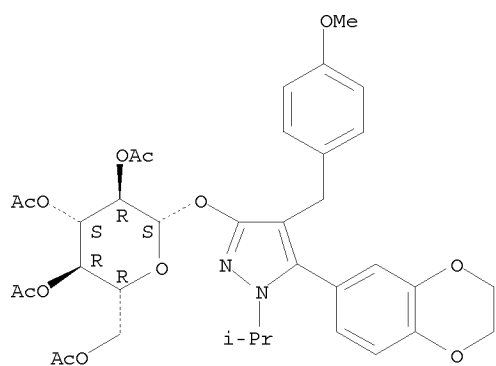
10/529,895



RN 678994-96-2 CAPLUS

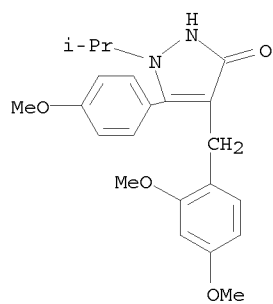
CN β -D-Glucopyranoside, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl, 2,3,4,6-tetraacetate (CA INDEX NAME)

Absolute stereochemistry.



RN 678994-98-4 CAPLUS

CN 3H-Pyrazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-1,2-dihydro-5-(4-methoxyphenyl)-1-(1-methylethyl)- (CA INDEX NAME)



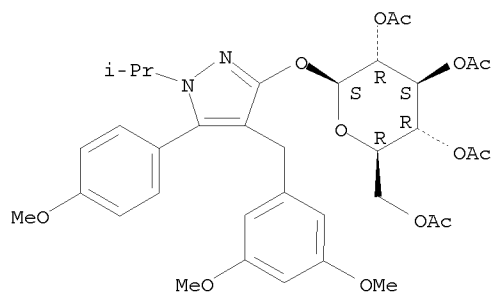
RN 678995-00-1 CAPLUS

CN β -D-Glucopyranoside, 4-[(3,5-dimethoxyphenyl)methyl]-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl, 2,3,4,6-tetraacetate (CA INDEX NAME)

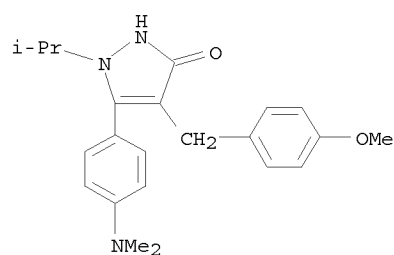
Absolute stereochemistry.

McIntosh

10/529,895



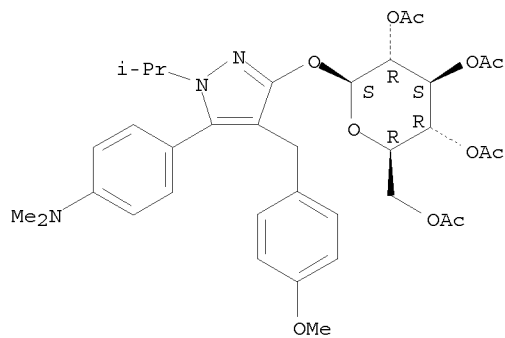
RN 678995-09-0 CAPLUS
CN 3H-Pyrazol-3-one, 5-[4-(dimethylamino)phenyl]-1,2-dihydro-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 678995-10-3 CAPLUS
CN β-D-Glucopyranoside, 5-[4-(dimethylamino)phenyl]-4-[(4-methoxyphenyl)methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl, 2,3,4,6-tetraacetate (CA INDEX NAME)

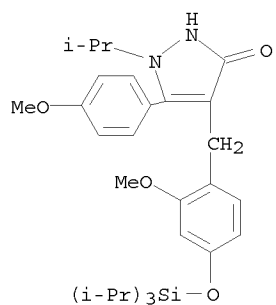
Absolute stereochemistry.



RN 678995-13-6 CAPLUS
CN 3H-Pyrazol-3-one, 1,2-dihydro-5-(4-methoxyphenyl)-4-[[2-methoxy-4-[[tris(1-methylethyl)silyl]oxy]phenyl)methyl]-1-(1-methylethyl)- (CA INDEX NAME)

McIntosh

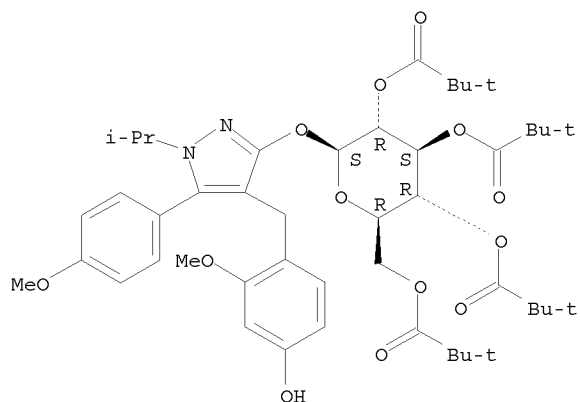
10/529,895



RN 678995-14-7 CAPLUS

CN β -D-Glucopyranoside, 4-[(4-hydroxy-2-methoxyphenyl)methyl]-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl, 2,3,4,6-tetrakis(2,2-dimethylpropanoate) (CA INDEX NAME)

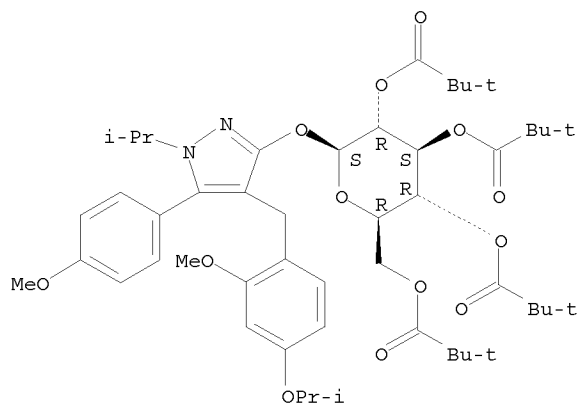
Absolute stereochemistry.



RN 678995-15-8 CAPLUS

CN β -D-Glucopyranoside, 4-[[2-methoxy-4-(1-methylethoxy)phenyl]methyl]-5-(4-methoxyphenyl)-1-(1-methylethyl)-1H-pyrazol-3-yl, 2,3,4,6-tetrakis(2,2-dimethylpropanoate) (CA INDEX NAME)

Absolute stereochemistry.



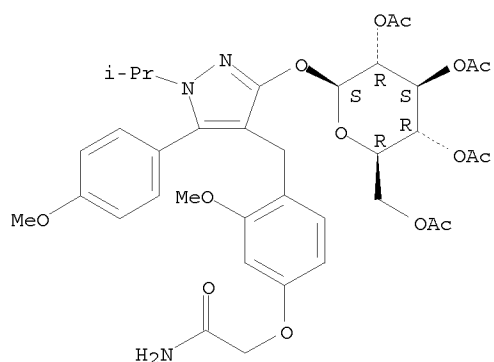
RN 678995-16-9 CAPLUS

CN Acetamide, 2-[3-methoxy-4-[[5-(4-methoxyphenyl)-1-(1-methylethyl)-3-[(2,3,4,6-tetra-O-acetyl-beta-D-glucopyranosyl)oxy]-1H-pyrazol-4-yl]methyl]phenoxy]- (CA INDEX NAME)

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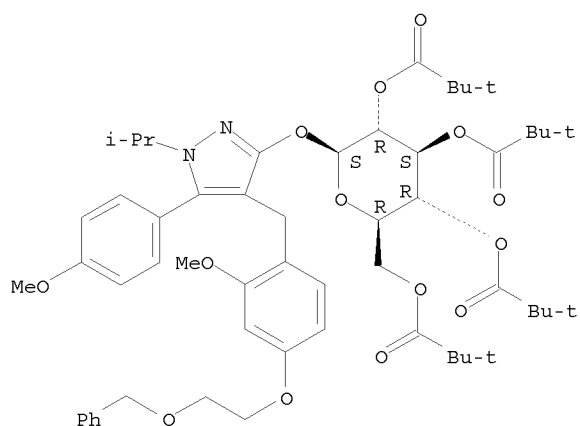
Absolute stereochemistry.



RN 678995-17-0 CAPLUS

CN β -D-Glucopyranoside, 5-(4-methoxyphenyl)-4-[[2-methoxy-4-[2-(phenylmethoxy)ethoxy]phenyl]methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl, 2,3,4,6-tetrakis(2,2-dimethylpropanoate) (CA INDEX NAME)

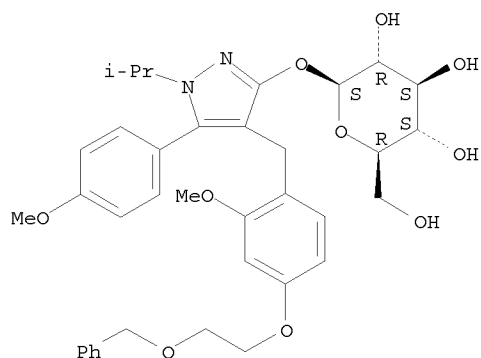
Absolute stereochemistry.



RN 678995-18-1 CAPLUS

CN β -D-Glucopyranoside, 5-(4-methoxyphenyl)-4-[[2-methoxy-4-[2-(phenylmethoxy)ethoxy]phenyl]methyl]-1-(1-methylethyl)-1H-pyrazol-3-yl (CA INDEX NAME)

Absolute stereochemistry.

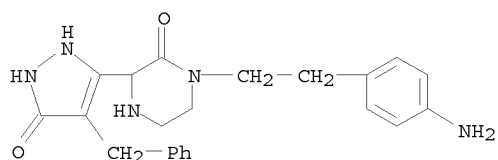


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RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2001:560439 CAPLUS
DN 135:338686
TI Similarity searching in large combinatorial chemistry spaces
AU Rarey, Matthias; Stahl, Martin
CS GMD-German National Research Center for Information Technology, Institute
for Algorithms and Scientific Computing (SCAI), Sankt Augustin, 53754,
Germany
SO Journal of Computer-Aided Molecular Design (2001), 15(6), 497-520
CODEN: JCADEQ; ISSN: 0920-654X
PB Kluwer Academic Publishers
DT Journal
LA English
AB We present a novel algorithm, called Ftrees-FS, for similarity searching
in large chemical spaces based on dynamic programming. Given a query compound,
the algorithm generates sets of compds. from a given chemical space that are
similar to the query. The similarity search is based on the feature tree
similarity measure representing mols. by tree structures. This descriptor
allows handling combinatorial chemical spaces as a whole instead of looking
at subsets of enumerated compds. Within few minutes of computing time,
the algorithm is able to find the most similar compound in very large spaces
as well as sets of compds. at an arbitrary similarity level. In addition,
the diversity among the generated compds. can be controlled. A set of
17,000 fragments of known drugs, generated by the RECAP procedure from the
World Drug Index, was used as the search chemical space. These fragments can
be combined to more than 1018 compds. of reasonable size. For validation,
known antagonists/inhibitors of several targets including dopamine D4,
histamine H1, and COX2 are used as queries. Comparison of the compds.
created by Ftrees-FS to other known actives demonstrates the ability of
the method to jump between structurally unrelated mol. classes.
IT 371974-30-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); MSC (Miscellaneous); PRP (Properties); BIOL
(Biological study)
(search for thrombin inhibitors; similarity searching in large
combinatorial chemical spaces)
RN 371974-30-0 CAPLUS
CN 2-Piperazinone, 1-[2-(4-aminophenyl)ethyl]-3-[2,5-dihydro-5-oxo-4-
(phenylmethyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

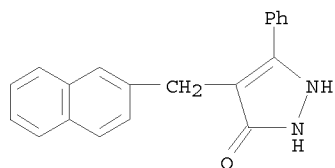


RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

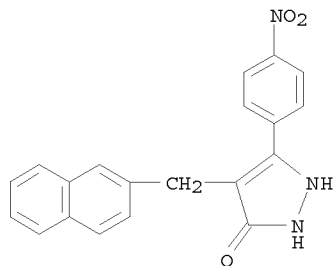
L19 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1995:352125 CAPLUS
DN 123:169535
OREF 123:30267a,30270a
TI Studies on New Acidic Azoles as Glucose-Lowering Agents in Obese, Diabetic
db/db Mice
AU Kees, Kenneth L.; Caggiano, Thomas J.; Steiner, Kurt E.; Fitzgerald, John
J., Jr.; Kates, Michael J.; Christos, Thomas E.; Kulishoff, John M.;
Moore, Robin D.; McCaleb, Michael L.
CS Wyeth-Ayerst Research, Princeton, NJ, 08543-8000, USA
SO Journal of Medicinal Chemistry (1995), 38(4), 617-28
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 123:169535
AB Bioisosteric substitution was used as a tool to generate several new

structural alternatives to the thiazolidine-2,4-dione and tetrazole heterocycles as potential antidiabetic agents. Among the initial leads that emerged from this strategy, a family of acidic azoles, isoxazol-3- and -5-ones and a pyrazol-3-one, showed significant plasma glucose-lowering activity (17-42% reduction) in genetically obese, diabetic db/db mice at a dose of 100 mg/kg/day +4. Structure-activity relationship studies determined that 5-alkyl-4-(arylmethyl)pyrazol-3-ones, which exist in solution as aromatic enol/iminol tautomers, were the most promising new class of potential antidiabetic agent (32-45% reduction at 20 mg/kg/d +4). Included in this work are convenient syntheses for several types of acidic azoles that may find use as new acidic bioisosteres in medicinal chemical such as the antidiabetic lead 5-(trifluoromethyl)pyrazol-3-one, hydroxy tautomer, and aza homologs of the pyrazolones, 1,2,3-triazol-5-ones (hydroxy tautomer) and 1,2,3,4-tetrazol-5-one heterocycles. Log P and pKa data for 15 potential acidic bioisosteres, all appended to a 2-naphthalenylmethyl residue so as to maintain a similar distance between the acidic hydrogen and arene nucleus, are presented. This new data set allows comparison of a wide variety of potential acid mimetics (pKa 3.78-10.66; log P -0.21 to 2.76) for future drug design.

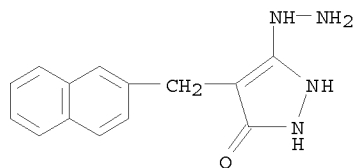
IT 164296-01-9P 164296-03-1P 164296-04-2P
 164296-13-3P 164300-88-3P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation of acidic azoles as glucose-lowering agents in obese, diabetic db/db mice)
 RN 164296-01-9 CAPLUS
 CN 3H-Pyrazol-3-one, 1,2-dihydro-4-(2-naphthalenylmethyl)-5-phenyl- (CA INDEX NAME)



RN 164296-03-1 CAPLUS
 CN 3H-Pyrazol-3-one, 1,2-dihydro-4-(2-naphthalenylmethyl)-5-(4-nitrophenyl)- (CA INDEX NAME)

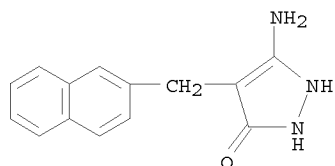


RN 164296-04-2 CAPLUS
 CN 3H-Pyrazol-3-one, 5-hydrazino-1,2-dihydro-4-(2-naphthalenylmethyl)- (9CI) (CA INDEX NAME)

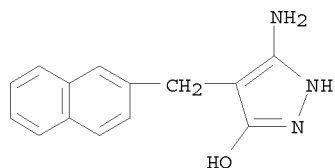


10/529,895

RN 164296-13-3 CAPLUS
CN 3H-Pyrazol-3-one, 5-amino-1,2-dihydro-4-(2-naphthalenylmethyl)- (CA INDEX NAME)

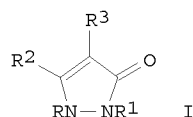


RN 164300-88-3 CAPLUS
CN 1H-Pyrazol-3-ol, 5-amino-4-(2-naphthalenylmethyl)- (CA INDEX NAME)



L19 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1984:209808 CAPLUS
DN 100:209808
OREF 100:31863a,31866a
TI 5-Pyrazolone derivatives useful in the treatment of cardiac insufficiency
IN Jarreau, Francois Xavier; Koenig, Jean Jacques
PA Etablissements Nativelle S. A., Fr.
SO Fr. Demande, 14 pp.
CODEN: FRXXBL
DT Patent
LA French
FAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE

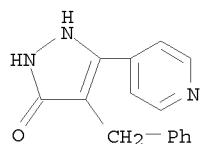
PI FR 2529786 A1 19840113 FR 1982-12177 19820712
FR 2529786 B1 19850111
PRAI FR 1982-12177 19820712
OS CASREACT 100:209808; MARPAT 100:209808
GI



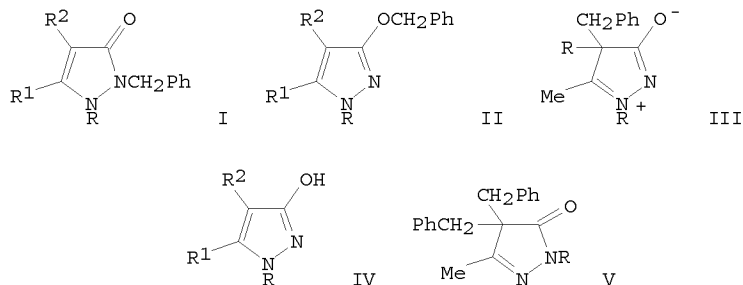
AB Pyrazolones I (R and R1 are H, alkyl; R2 = Ph, alkylphenyl, pyridyl, alkylpyridyl; R3 = H, alkyl, Ph, aralkyl) which showed cardiovascular activity, were prepared from the resp. RNHNHR1 and R2COCHR3CO2Et. Thus, EtOAc, Et isonicotinate, and NaH gave Et isonicotinoylacetate, and the latter was treated with N2H4 to give I (R2 = 4-pyridyl, R = R1 = R3 = H).
IT 90280-29-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 90280-29-8 CAPLUS
CN 3H-Pyrazol-3-one, 1,2-dihydro-4-(phenylmethyl)-5-(4-pyridinyl)- (CA INDEX NAME)

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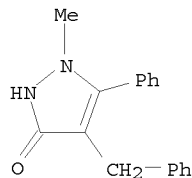


L19 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1981:515384 CAPLUS
DN 95:115384
OREF 95:19361a,19364a
TI Photochemical benzyl migration in 3-pyrazolin-5-ones
AU Singh, Gurbakhsh; Singh, Devender; Ram, Ram Nath
CS Univ. Delhi, Delhi, India
SO Tetrahedron Letters (1981), 22(23), 2213-16
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 95:115384
GI



AB The pyrazolinones I (R = R1 = Me, R2 = H, Me, PhCH2; R = Me, R1 = Ph, R2 = H; R = CH2Ph, R1 = Me, R2 = H) on irradiation underwent N→O and N→C-4 benzyl migrations to give 18-25% benzyloxypyrazoles II and the betaines III (R = Me, CH2Ph) (56 and 27%, resp.) or, owing to a subsequent prototropic shift, 18-25% hydroxypyrazoles IV (R = Me, R1 = Me, Ph; R = CH2Ph, R1 = Me; R2 = PhCH2), resp. IV (R = R1 = Me, R2 = H, Me, CH2Ph; R = Me, R1 = Ph, R2 = H; R = CH2Ph, R1 = Me, R2 = H) were also formed (16-32%) by fragmentation followed by H abstraction. I (R = CH2Ph, R1 = Me, R2 = H) also gave V (R = CH2Ph, H) (14 and 10%, resp.). A free-radical mechanism is proposed.

IT 79000-07-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 79000-07-0 CAPLUS
CN 3H-Pyrazol-3-one, 1,2-dihydro-1-methyl-5-phenyl-4-(phenylmethyl)- (CA INDEX NAME)

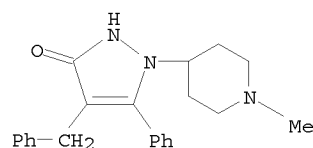


L19 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1962:429631 CAPLUS

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10/529,895

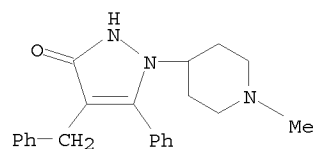
DN 57:29631
OREF 57:5905d-f
TI Determination of the structure of an isomer occurring in the preparation of 1-(N-methyl-4-piperidyl)-3-phenyl-4-benzyl-5-pyrazolone as 1-(N-methyl-4-piperidyl)-4-benzyl-5-phenyl-3-pyrazolone. I. Communication on x-ray structure analysis
AU Leemann, H. G.; Antenen, K.
CS Sandoz A.-G., Basel, Switz.
SO Helvetica Chimica Acta (1962), 45, 177-9
CODEN: HCACAV; ISSN: 0018-019X
DT Journal
LA German
GI For diagram(s), see printed CA Issue.
AB In the manufacture of the title compound (Swiss 346,886; Ebnoether, et al., CA 54, 22589b; Jucker and Lindenmann CA 56 1532i) there was formed a small amount of an isomer, for which 5 structures were conceivable. On the basis of formation of a monomethiodide (I), 284-6° (decomposition) (MeOH), various phys.-chemical measurements, and x-ray structure analysis of I, the isomer had structure II.
IT 95226-83-8P, 3-Pyrazolin-5-one, 4-benzyl-2-(1-methyl-4-piperidyl)-3-phenyl- 100659-82-3P, 3-Pyrazolin-5-one, 4-benzyl-2-(1-methyl-4-piperidyl)-3-phenyl-, methiodide
RL: PREP (Preparation)
(preparation of)
RN 95226-83-8 CAPLUS
CN 3-Pyrazolin-5-one, 4-benzyl-2-(1-methyl-4-piperidyl)-3-phenyl- (7CI) (CA INDEX NAME)



RN 100659-82-3 CAPLUS
CN 3-Pyrazolin-5-one, 4-benzyl-2-(1-methyl-4-piperidyl)-3-phenyl-, methiodide (7CI) (CA INDEX NAME)

CM 1

CRN 95226-83-8
CMF C22 H25 N3 O



CM 2

CRN 74-88-4
CMF C H3 I

H₃C-I

L19 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1954:56650 CAPLUS
DN 48:56650
OREF 48:10009b-i,10010a-d
TI Pyrazolones

McIntosh

AU Gagnon, Paul E.; Boivin, Jean L.; Tremblay, Meude
 CS Laval Univ., QC
 SO Canadian Journal of Chemistry (1953), 31, 673-84
 CODEN: CJCHAG; ISSN: 0008-4042

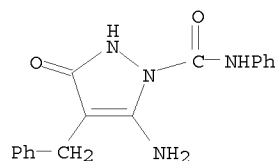
DT Journal

LA Unavailable

AB 1,4-Diphenyl-3-carbethoxy-5-aminopyrazole (I) gives 1,4-diphenyl-5-aminopyrazole (II) on hydrolysis and decarboxylation. Thus, 1.0 g. I and 50 ml. 10% NaOH in 25 ml. absolute EtOH refluxed 3 hrs., the solution is poured in ice-H₂O, neutralized with dilute AcOH, filtered, and the filtrate acidified with HCl to pH 3 gives 1,4-diphenyl-3-carboxy-5-aminopyrazole (III). III (1.1 g.) heated 45 min. at 200° until all the CO₂ is expelled gives II. EtO₂CCHPhC(:NNHPh)CO₂Et (IV) in alkali formed 1,4-diphenyl-3-carbethoxy-2-pyrazolin-5-one (V), saponified to 3-HO₂C analog (VI) and decarboxylated to 1,4-diphenyl-2-pyrazolin-5-one (VII). Thus 33.5 g. EtO₂CCHPhCOCO₂Et and 10.8 g. PhNHNH₂ heated 1 hr. on a steam bath and 2 hrs. in an oil bath at 210°, and the product dissolved in EtOH and poured into dilute alkali, filtered, and the filtrate acidified with AcOH give V. V (4.0 g.) heated 1 hr. with alc. KOH, poured into ice H₂O, and acidified with excess HCl gives VI. VI heated in a metal bath 0.5 hr. at 200° gives VII. A Curtius degradation on V is made through the hydrazide (VIII), azide (IX), and urethan (X); alkaline hydrolysis of X yields 1,4-diphenyl-3-amino-2-pyrazolin-5-one (XI). Thus, 7.7 g. V and 10 ml. 100% N₂H₄.H₂O refluxed 6 hrs., the mixture evaporated to dryness, and the residue dissolved in cold HCl neutralized with NaOH yields VIII. To VIII in HCl and Et₂O cooled to 0°, NaNO₂ in H₂O is added dropwise, and the Et₂O layer decanted, washed with 10% NaHCO₃, dried over Na₂SO₄, and evaporated in vacuo to give IX. IX refluxed 20 hrs. in absolute EtOH forms X. X (0.6 g.) treated 3 hrs. with 10% NaOH, cooled, filtered, treated with HOAc, the precipitate dissolved in Et₂O, the solution dried with Na₂SO₄, and evaporated to dryness gives XI. 2,4-Diphenyl-3-hydroxy-2-pyrazolin-5-one (XII) is obtained by adding 11.8 g. PhCH(CO₂Et)₂ and 5.4 g. PhNHNH₂ to a cold solution of 2.4 g. Na in 75 ml. absolute EtOH, refluxing 18 hrs. and evaporating the EtOH in vacuo. PhCH(CN)CONHNHPh (4.2 g.) and 50 ml. glacial AcOH refluxed 72 hrs., the mixture cooled, the crystalline solid dissolved in 400 ml. 5% cold NaOH solution, filtered, and the filtrate acidified with AcOH forms 2,4-diphenyl-3-amino-2-pyrazolin-5-one (XIII). The compds. prepared by the above methods have the following consts. (m.p., and ultraviolet absorption maximum in A. (log Em) in neutral and in acid solution, resp., given): V, 142-3°, 2410 (4.32); 2450 (4.27). VI, 192-3°, 2440 (4.40); 2450 (4.34). VII, 196-7°, 2550 (4.34), 2830 (4.18); 2440 (4.16). VIII, 203-4°, 2400 (4.50); 2420 (4.52). X, 193-4°, 2520 (4.31), 3050 (3.50); 2510 (4.38), 2980 (3.49). XI, 153-6° (decomposition), 2560 (4.26); 2540 (4.20). XII, 172-3°, 2350 (4.18), 2820 (3.30); 2340 (4.16), 2800 (3.31). XIII, 234-6°, 2800 (4.26); 2500 (4.18). 4-Monosubstituted 3-hydroxy-2-pyrazolin-5-ones are formed when 0.033 mole Et monosubstituted-malonates and 0.033 mole hydrazine derivs., 4-PhNHCONHNH₂ or 1- or 2-ClO₂H₇NHNH₂.HCl, are refluxed 18 hrs. with 0.10 mole Na in 75 ml. absolute EtOH, the EtOH is evaporated, the residues dissolved in H₂O, the solution extracted with Et₂O, filtered, and the aqueous layer acidified with 50% AcOH. Thus 4-substituted 3-hydroxy-2-carbanilino-2-pyrazolin-5-ones (XIV) are prepared (4-substituent, m.p., and ultraviolet absorption maximum in A. (log Em) in neutral and in acid solution, resp. are given): C₆H₁₃, 170-1° (decomposition), 2380 (4.05); 2370 (3.99). C₇H₁₅, 160-2° (decomposition), 2380 (4.20); 2380 (4.10). C₈H₁₇, 150-1°, 2540 (4.37); 2540 (4.38). Also 4-alkyl-3-hydroxy-2-(α- or β-naphthyl)-2-pyrazolin-5-ones (XV) (4-substituent, α or β, m.p., and ultraviolet absorption data given): C₈H₁₇, α, 184-5°, 2400 (4.32), 3140 (3.74); 2380 (4.29), 3050 (3.74). PhCH₂, α, 169-170°, 2230 (4.76), 2770 (3.88); 2235 (4.71), 2810 (3.94). C₄H₉, β, 172-3°, 2440 (4.45), 2975 (4.28); 2320 (4.67), 3010 (3.90). C₅H₁₁, β, 157-8°, 2440 (4.47), 2980 (4.01); 2330 (4.61), 2940 (3.92). C₆H₁₃, β, 155-6°, 2270, 4.54, 2890, 3.92; 2310, 4.61, 3000, 3.90. C₇H₁₆, β, 152-3°, 2450 (4.45), 3000 (4.00); 2320 (4.52), 2990 (3.88). C₈H₁₇, β, 147-8°, 3000 (3.97); 2340 (4.61), 3000 (3.89). PhCH₂, β, 189-90°, 2350 (4.53), 3000 (3.75); 3000, 3.79. The 4-monosubstituted-3-amino-2-carbanilino-2-pyrazolin-5-ones (XVI) are prepared in the same way as XIV and XV except that the Et monosubstituted-malonates are replaced by ethyl monosubstituted-cyanoacetates (4-substituent, m.p., and ultraviolet data): C₄H₉, 117-18°, 2380 (4.22); 2420 (4.30). C₅H₁₁, 115-16°, 2480 (4.34); 2380 (4.24). C₆H₁₃, 113-14°, 2420 (4.50); 2370 (4.22).

C7H15, 110-11°, 2450 (4.33); 2400 (4.28). C8H17, 264-5°, 2460 (4.18), 2920 (3.68); 2430 (4.30), 2840 (3.77). PhCH2, 240-5°, 2880 (3.79); 2790 (3.73). 4,4-Disubstituted-3,5-pyrazolinediones (XVII) are prepared in the same way from Et disubstituted-malonates and PhNHCONHNH2 or 2-ClOH7NHNH2.HCl (4- and 2-substituents, m.p., and ultraviolet absorption data given): (C4H9)2, PhNHCO, 217-18°, 2550 (3.74); 2520 (3.81). (C6H13)2, PhNHCO, 198-9°, 2530 (3.74); 2510 (3.77). (C7H15)2, PhNHCO, 199-200°, 2510 (3.72); 2450 (3.83). (C8H17)2, PhNHCO, 194-5°, 2530 (3.69); 2520 (3.75). (PhCH2)2, PhNHCO, 243-5°, 2400 (3.39); 2400 (4.41). (PhCH2)2, 2-ClOH7, 243-4°, 2990 (3.89); 2970 (3.89). Et dialkylcyanoacetates are treated with PhNHCONHNH2 as for XV to yield 4,4-disubstituted-3-imino-2-carbanilino-5-pyrazolidinones (XVIII) (4-substituents, m.p., and ultraviolet absorption data given): (C4H9)2, 234-6°, -. (C5H11)2, 95-7°, 2460 (4.48); 2400 (4.25). (C6H13)2, 100-2°, 2450 (4.54); 2380 (4.15). (C8H17)2, 167-8°, 2700 (3.82); 2660 (3.89). The structures of the various pyrazolidinones are interpreted from the ultraviolet absorption data.

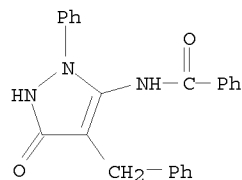
IT 857182-23-1P, 3-Pyrazoline-2-carboxanilide, 3-amino-4-benzyl-5-oxo-
RL: PREP (Preparation)
(preparation of)
RN 857182-23-1 CAPLUS
CN 1H-Pyrazole-1-carboxamide, 5-amino-2,3-dihydro-3-oxo-N-phenyl-4-
(phenylmethyl)- (CA INDEX NAME)



L19 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1951:60116 CAPLUS
DN 45:60116
OREF 45:10239f-i,10240a-h
TI The synthesis and ultraviolet spectra of some pyrazolones
AU Gagnon, Paul E.; Boivin, Jean L.; Boivin, Paul A.; Jones, R. Norman
CS Laval Univ., QC
SO Canadian Journal of Chemistry (1951), 29, 182-91
CODEN: CJCHAG; ISSN: 0008-4042
DT Journal
LA Unavailable
AB cf. C.A. 44, 5874b. NCCH2CO2Et (I) (113 g.) and 98.5 g. PhCH:CHCH2Br, added to a solution of 11.5 g. Na in 200 ml. absolute EtOH, the mixture refluxed 2 hrs., the EtOH removed, the residue shaken with H2O and then Et2O, and the dried Et2O extract fractionally distilled, gave 68.7 g. (60%) Et α -cyano- α -cinnamylacetate (II), b12 206-8°. II (22.9 g.) stirred (heat evolved) 5 min. with 5.0 g. 100% N2H4.H2O (III) produced a quant. yield of α -cyano- α -cinnamylacetohydrazide (IV), white solid, m. 94-5° (from EtOH) (all m.ps. uncor.). Treatment of IV and 3 other monosubstituted cyanoacetohydrazides with strong alkali according to G., et al. (C.A. 43, 7477i), produced a series of the corresponding 4-monosubstituted-3-amino-5-pyrazolones: nonyl, m. 222-3°; stearyl, m. 200-2°; 2-cyclohexylethyl, m. 203-5°; cinnamyl, m. 198-200°. Three 4-monosubstituted-3-amino-2-phenyl-5-pyrazolones (nonyl, m. 167-8°; Ac (V), m. 217-19°; 2-cyclohexylethyl, m. 154-5°) were prepared by heating the corresponding monosubstituted I with PhNHNH2 (VI) and NaOEt. 4-(1-Naphthyl)-3-amino-2-carbamyl-5-pyrazolone (VII), m. 273-5°, prepared similarly but by heating 18 hrs. with NH2CONHNH2 (VIII)-HCl, was soluble in alkalis and strong acids, insol. in Na2CO3, and precipitated from its alkaline solution by CO2. A series of Et dialkylcyanoacetates was prepared by adding 0.5 equivalent I and 1 equivalent organic halide to a cooled solution of 1 mole Na in 400 ml. absolute EtOH, refluxing until the mixture was neutral, removing the EtOH, pouring the residue into cold H2O, and fractionating the Et2O extract, which had been previously washed with 5% NaOH and then dried over Na2SO4 (read alkyl group, yield in %, b.p./mm.): 1-methylbutyl, 50, 153-6°/13; hexyl, 50, 176-8°/13; heptyl, 51,

198-201°/13; octyl, 48, 152-5°/6; nonyl, 45, 170-4°/6. These and 3 other Et dialkylcyanoacetates (0.1 mole of each), separately heated 24 hrs. in an oil bath at 160° with 0.1 mole VIII.HCl and a solution of 0.3 mole Na in 120 ml. absolute EtOH, the solvent removed, the residue dissolved in 100 ml. hot H₂O, extracted with Et₂O (to remove unchanged esters), and the aqueous solution acidified (AcOH), gave the corresponding 4,4-dialkyl-5-imino-1-carbamyl-3-pyrazolidones (di-Pr, m. 304-7°; di-Bu, m. 278-80°; bis(1-methylbutyl), m. 300°; di-Am (IX), m. 273-5°; dihexyl, m. 261-3°; diheptyl, m. 270-2°; dioctyl, m. 266-8°; dinonyl, m. 259-61°), which were crystallized from EtOH or AcOH and were soluble in alkalies, insol. in strong acids, and were precipitated from alkaline solution by CO₂. That VI with substituted I forms 2-phenylpyrazolones and with unsubstituted I forms 1-phenylpyrazolones was demonstrated by the following unambiguous synthesis of 4-benzyl-3-amino-1-phenyl-5-pyrazolone (X) and by showing the Bz derivative (XI) of X to be different from that (XII) of the corresponding 2-Ph isomer (XIII). VIII is considered to react like VI with substituted I and thus to form 2-carbamyl-5-pyrazolones. VI (10.8 g.) was added (heat evolved) to 27.8 g. EtO₂CCOCH(CH₂Ph)CO₂Et, the mixture heated 1 hr. on a steam bath (H₂O formed), then gradually to 210° (EtOH evolved), and the solid residue crystallized from EtOH to yield 95% 4-benzyl-3-carbethoxy-1-phenyl-5-pyrazolone (XIV), m. 194-5°, also obtained in low yield according to Munzesheimer and Wislicenus [Ber. 31, 554(1898)]. XIV (32.2 g.) was unaffected by aqueous KOH but, heated 1 hr. on a steam bath with alc. KOH and the mixture poured into 600 ml. ice-water and strongly acidified with 50% HCl, it gave the white 4-benzyl-3-carboxy-1-phenyl-5-pyrazolone (XV), m. 233-4° (from EtOH). XV (29.4 g.), heated 1 hr. on a H₂O bath with 28 ml. SOCl₂ and the excess SOCl₂ evaporated (reduced pressure), gave the corresponding acid chloride (XVI), brown viscous liquid. XVI (20 g.) in 300 ml. Et₂O, added to 20 g. NaN₃ in 30 ml. H₂O, the mixture stirred 2 hrs. in an ice bath, the Et₂O decanted, washed with Na₂CO₃ and then ice water, dried (Na₂SO₄), poured into absolute EtOH, the Et₂O distilled (N evolved), and the alc. solution boiled 12 hrs. and cooled overnight, gave 4-benzyl-3-carbethoxyamino-1-phenyl-5-pyrazolone (XVII), m. 178-9° (from EtOH). XVII (2 g.), refluxed 2 hrs. with NaOH and the solution neutralized with AcOH, yielded the white X, m. 206-7° (from EtOH). X (2 g.), heated 18 hrs. on a H₂O bath in 25 ml. dry dioxane with 2 ml. BzCl, the excess BzCl removed (reduced pressure), and the residue recrystd. twice from EtOH gave XI, m. 225-7°. Similarly was prepared XII, m. 197-8° (from EtOH). XVII also was prepared from the hydrazide (XVIII). Thus, 16.1 g. XIV, heated 6 hrs. (EtOH formed) at 140° with 16 ml. III, the mixture poured into 400 ml. H₂O, neutralized with AcOH, the white solid treated at 0° with concentrated HCl, and the acid filtrate neutralized at 0° with 5% NaOH, produced XVIII, brown resinous material, very soluble in EtOH, Et₂O, and C₆H₆, which could not be crystallized. XVIII in HCl, extracted with Et₂O (to remove impurities), covered with 200 ml. Et₂O, cooled to 0°, stirred 2 hrs. while NaNO₂ in H₂O was added dropwise, the Et₂O decanted, the aqueous layer extracted 3 times with Et₂O, and the combined exts. washed (Na₂CO₃), dried (Na₂SO₄), and a portion evaporated, yielded the crystalline azide, m. 134° (with deflagration). The remainder of the Et₂O extract, poured into 200 ml. EtOH, the Et₂O removed through a fractionating column, and the alc. solution boiled 12 hrs. and then concentrated, gave XVII, m.p. and mixed m.p. with the above sample 178-9°. Ultraviolet absorption spectra are reproduced graphically for X, XIII, V, VII, and IX in neutral (95% EtOH) and acid (0.1 N HCl in 95% EtOH) solns. (also in alkaline solution for IX), and the absorption maximum and log E_{maximum} values for the first 16 pyrazolones cited in this abstract are tabulated for neutral and acid solns. The spectrum of XIII shifts to longer wave lengths on acidification while that of X remains unchanged.

IT 859296-48-3P, 3-Pyrazolin-5-one, 3-benzamido-4-benzyl-2-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 859296-48-3 CAPLUS
 CN Benzamide, N-[2,5-dihydro-5-oxo-2-phenyl-4-(phenylmethyl)-1H-pyrazol-3-yl]-
 (CA INDEX NAME)



L19 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1951:47007 CAPLUS
 DN 45:47007
 OREF 45:8009i,8010a-b
 TI 4-Monosubstituted-3-amino-5-pyrazolones
 AU Gagnon, Paul E.; Boivin, Jean L.; Giguere, Jacques
 CS Laval Univ., QC
 SO Canadian Journal of Chemistry (1951), 29, 328-32
 CODEN: CJCHAG; ISSN: 0008-4042
 DT Journal
 LA Unavailable
 AB The hydrazide (0.1 mol.) of an alkyl-substituted cyanoacetic acid was treated with 2 equivs. NaOH (40%), stirred several min., kept 3 hrs., diluted with 250 ml. H₂O, and acidified with 50% AcOH to give the pyrazolone, which was recrystd. several times from aqueous EtOH. The yields were excellent. All of the compds. gave a pos. color test with aqueous FeCl₃. The following 4-substituted 3-amino-5-pyrazolones were prepared (m.p. given): dodecyl 152-4°, o-chlorobenzyl 170°, 2-(p-methylphenoxy)ethyl 184-5°, 3-(p-methylphenoxy)propyl 159-60°, 2-(p-ethylphenoxy)ethyl 170-1°, 2-(p-chlorophenoxy)ethyl 204-5°, 3-(p-chlorophenoxy)propyl 203-4°, and 3-(p-bromophenoxy)propyl 214-16°. The ultraviolet absorption spectra of these compds. were taken in neutral, acid, and alkaline media; the hypsochromic displacement in acid and alkaline media is explained on the basis of the existence of tautomeric forms.
 IT 857988-95-5P, 3-Pyrazolin-5-one, 3-amino-4-o-chlorobenzyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 857988-95-5 CAPLUS
 CN 3H-Pyrazol-3-one, 5-amino-4-[(2-chlorophenyl)methyl]-1,2-dihydro- (CA INDEX NAME)

